IBIS

Final Report

Lowest Foreseeable Cost
of CVD Diamond

Contract Number: N00014-93-C2044

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Executive Summary

IBIS Associates has completed its predictive spreadsheet models of chemical vapor deposition (CVD) diamond film fabrication. This report details the capabilities of the models, and shows cost sensitivities to product and process input parameters, in order to assess the lowest foreseeable cost of CVD diamond.

For this report and the results contained herein, it is assumed that the transport theory model, which predicts growth rates in the CVD diamond technical cost models, closely predicts actual growth rates for the deposition technologies and that the input values for variables such as the gas flow rate and substrate diameter are physically achievable.

According to the IBIS Technical Cost Models (TCMs), the cost of CVD diamond will reach the $4 per carat level in the five to ten year outlook. Achieving this cost level are the DC arcjet and microwave technologies, as modeled in this program. While the combustion flame technology may attain this cost level with alternative implementations (i.e., different gases or nozzle geometries), the IBIS TCMs show a lower boundary for this technology at about $20 per carat.

Looking beyond the five to ten year outlook, IBIS has analyzed the theoretical upper limit on growth rate as well as the likely upper limits on technology scaling, and has investigated the effect of these assumptions on deposition cost. Implemented as part of the DC arcjet technology, this cost modeling effort predicts cost levels of $0.42 per carat. Since such a diamond deposition machine would produce 3.1 million carats per year, it is assumed that a CVD diamond market of at least this size will exist.

Additionally, this final report summarizes the results of a survey conducted by IBIS Associates to solicit opinions on the future of CVD diamond. Similarities in the responses regarding process scaling suggest that organizations involved with CVD diamond plan to continue investment and cost reduction. Specific opinions are summarized in this report.

Lastly, this final report provides an overview of previous reports. As part of this program, IBIS has investigated the economics of diamond finishing (planarization). The summaries from these reports plot the progress of the IBIS cost modeling effort since the project's beginning in January, 1993.

Introduction

The international effort to manufacture and commercialize diamond has succeeded in making a commodity of diamond grit, but requires further progress to succeed in doing the same for diamond films. Diamond grit has been produced through methods developed over the past forty years, resulting in a product that has a low cost-to-performance ratio relative to competing materials. Diamond films have been produced through methods developed over only the past ten years, and progress to date has resulted in a product that has a high cost to performance ratio relative to competing materials. Table 1 lists competing materials for both diamond grit and films for different applications, along with the properties and order of magnitude prices for these materials.

Motivation for manufacturing diamond is driven by these properties listed in Table 1. Diamond's high hardness is desirable for abrasive applications: polishing slurries, bonded grit (e.g. grinding wheels), and polycrystalline film coatings (e.g. drills). With high hardness relative to the material being abraded, diamond tends to last longer while enabling higher operating speeds. Diamond's corrosion resistance enables operation with most materials and in most chemical environments.

This high resistance to wear, coupled with diamond's low coefficient of friction, makes diamond a desirable material for bearing applications. For use as a bearing, diamond would last longer than most materials while enabling higher efficiencies due to the reduced friction losses. Again, diamond's corrosion resistance provides an added attraction for its use.

Yet another quality, diamond's high thermal conductivity (low thermal resistance), is desirable for heat dissipation applications. In cases where heat generation sources such as resistive electronic circuits contact materials with high thermal resistance, thereby degrading product performance (i.e., slowing circuit operation), diamond allows lower temperatures and higher performance (i.e., faster signal transmission rates) through greater heat dissipation.

Additional benefits for electronic applications include diamond's coefficient of thermal expansion that matches well with silicon, the most widely used material in active electronic devices today, and diamond's high electrical resistance, allowing it to contact electronics directly. Lastly, the hardness and corrosion resistance enable diamond to be considered for harsh electronics operating conditions.

In another application of thermal dissipation, where heat is generated through friction, diamond's thermal conductivity can allow a lower temperature rise for a given friction heat source. This quality has utility for the sensor windows in aircraft and projectiles, where radiation is generated by the frictional heat on the sensor window surface. This radiation complicates the ability of the internal sensors to detect different sources of heat, such as

TABLE 1. Pricing and Properties of Electronic Materials

Property	CVD Diamond	Aluminum Nitride	Silicon	Copper	Alumina	Beryllia	Silicon Carbide
Density (g/cc)	3.5	3.3	2.3	8.9	3.9	3.0	2.5 - 3.2
Young's Modulus ($\times 10^{10}$ N/m^2)	110	35	11	12	39	38	45
Resistivity (Ohm-cm @ 25°C)	10^{12} - 10^{17}	10^{14}	3×10^5	2×10^{-4}	$>10^{15}$	$>10^{17}$	10^2 - 10^{12}
Coefficient of Thermal Expansion ($\times 10^{-6}$ / °C)	1 to 2	4	2.6	5.2	9	8	4
Thermal Conductivity (W/cm-K)	10 - 20	0.7 - 3	1.5	4	0.4	4	1 - 3
Dielectric Constant	5.6	9	11	N / A	9	7	40 - 100
Coefficient of Friction (on steel)	0.05 - 0.15	0.1 - 0.5	0.1 - 0.5	0.1 - 0.5	0.1 - 0.5	0.1 - 0.5	0.1 - 0.5
Vickers Hardness GPa	90	12	10	2	29	12 - 16	2 - 32
Order of Magnitude Price ($ per gram)	100 - 1,000	1 - 10	0.1 - 1	0.01 - 0.1	0.01 - 1	1 - 10	0.1 - 10

other aircraft and projectiles. With diamond as part of the sensor window, less heat and therefore less radiation would be generated to reduce the ability of the sensing devices. Also, diamond is optically transparent, allowing the optical portion of the electromagnetic spectrum to pass to the sensors unimpeded. Lastly, diamond's corrosion resistance allows operation under harsh conditions for this application.

While diamond films and grit could compete for certain abrasive applications, diamond films are being studied and developed for uses where diamond materials have not been possible to date. Such applications include the curved tool coatings, heat dissipation coatings and substrates, and sensor windows mentioned above.

Overall, diamond materials have improved many products and manufacturing processes in the case of high pressure, high temperature (HPHT) diamond grit, and will improve many new and existing products in the case of the newly developing chemical vapor deposited (CVD) diamond coatings. To date, only diamond grit has achieved widespread use for applications such as loose grit powder for abrasive uses and bonded grit for grinding wheels. The only barrier to widespread use for diamond film is price, although many organizations are developing cheaper polycrystalline diamond films. This report does not seek to compare the economics of diamond grit technology versus the diamond film deposition technology. Instead, this report focuses on the economic history and potential of CVD diamond, and it examines how CVD diamond technologies could lower manufacturing costs through process scaling.

Over the past five years, the costs of CVD diamond have decreased. The deposition costs have been reduced over this period due to both the technology advances and the increase in demand, as depicted in Figure 1. The reduction in manufacturing cost, although dramatic, is hampered by the different manufacturing conditions required by the many applications of this material. Ironically, the high number of applications has slowed the pace in reaching economies of scale for CVD diamond overall: the different applications require unique deposition conditions, and even equipment in some cases, that then translate to economies of scale reached only on a product-by-product basis. Progress in CVD diamond, therefore, has been spread over many development fronts.

Motivation for Cost Analysis

The commercial success of a new material depends on its cost and performance relative to its competitors. Since CVD diamond far outperforms the competition, the only barrier to its widespread use is its current cost, which is on the order of hundreds of dollars per carat. Even though potential users may be willing to pay more for synthetic diamond than other materials, the current price threshold for most organizations appears to be in the range of $1 to $5 per carat.

CVD Diamond Manufacturing Cost Vs. Time

Cost Per Carat: $1,000, $100, $10, $1

Year: 1988, 1990, 1992, 1994, 1996, 1998, 2000, 2002

Long Term Scenario
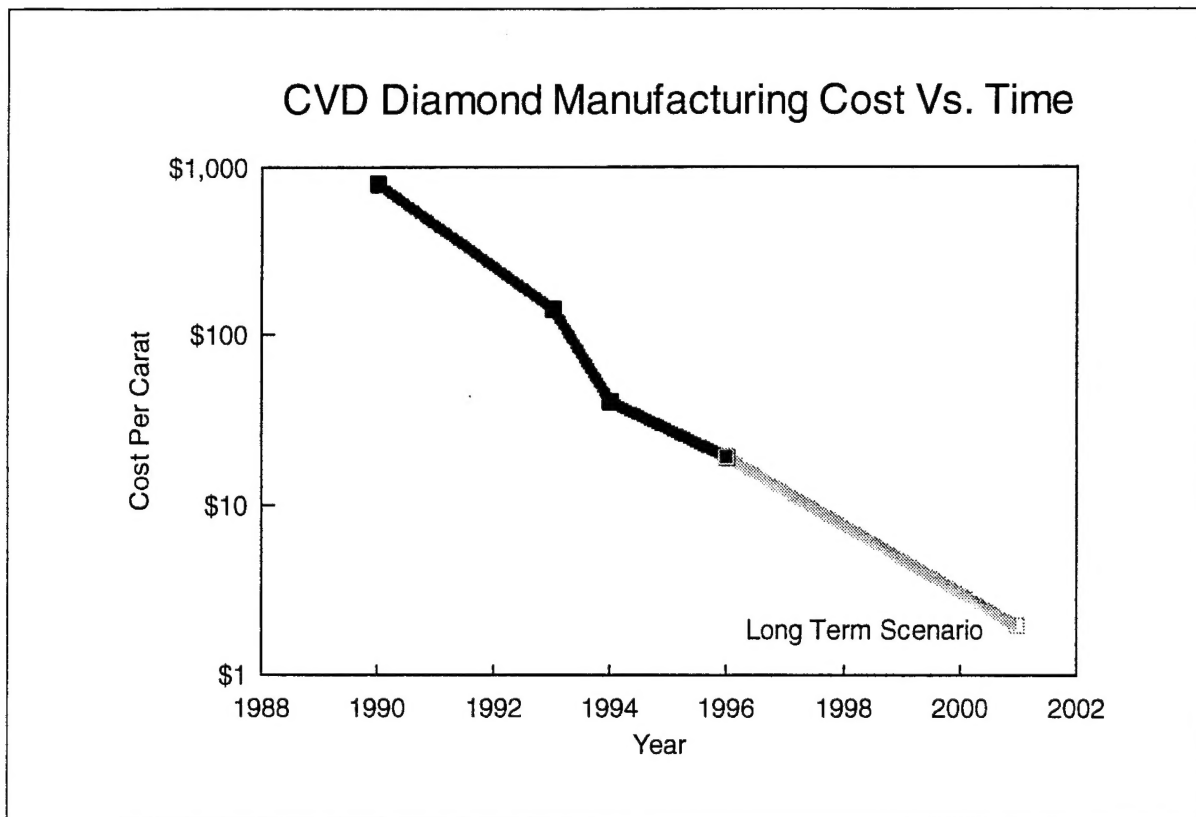
Figure 1. Progress of CVD Diamond

In achieving this cost goal, what technology changes must occur and to what extent? Answering this question is one of the strengths of Technical Cost Modeling. By focusing on cost as an important factor in technology development and identifying the cost "bottlenecks" for an operation (i.e., equipment throughput), companies can foresee lower costs, given the current understanding of the technology.

Methodology

The tool for cost prediction for this report is Technical Cost Modeling (TCM), a spreadsheet-based methodology for the estimation of manufacturing cost. In conjunction with TCM are predictive relationships that incorporate both empirical data and theoretical equations to provide model flexibility. This section details both the TCM methodology and the predictive relationships, and lists the inputs associated with the modeling performed in this report.

Technical Cost Modeling

Technical Cost Modeling is a tool for estimating and simulating manufacturing costs. The technique is an extension of conventional process modeling, with particular emphasis on capturing the cost implications of material and process variables and changing economic scenarios.

In a Technical Cost Model (TCM), cost is assigned to each unit operation from a process flow diagram. For each of these unit operations, total cost is broken down into separately calculated elements:

- Variable cost elements
  - *Material, labor, and utilities (energy)*
- Fixed cost elements
  - *Equipment, tooling, building*
  - *Maintenance, overhead labor, cost of capital*

By breaking cost down in this way, the complex task of cost estimation is reduced to a series of more simple engineering and economic calculations. A summary of the basic relationships in a Technical Cost Model is shown in Figure 2.

Technical Cost Models can be predictive in nature. In a predictive approach, parameters such as deposition rate and cycle time are calculated by the model as a function of the product material and geometry. These predictive functions can be derived from analysis of empirical data or through incorporation of theoretical relationships. It is this predictive nature of Technical Cost Models that enable their flexibility and subsequent utility.

Technical Cost Models can be used to accomplish tasks that include the following.

- Simulate the costs of manufacturing products
- Establish direct comparisons between material, process, and design alternatives
- Investigate the effect of changes in the process scenario on overall cost
- Identify limiting process steps and parameters
- Determine the merits of specific process and design improvements

Typical Technical Cost Model Logic

Product Inputs		Cost Summary
Geometry		
Materials		Variable Costs
Yield		Material
Equipment Inputs		Labor
Labor	Cycle Time	Utility
Utilities		
Rate		
Price		
Tooling		Fixed Costs
Floorspace		Equipment
		Tooling
		Building
Annual Production	Number of	Maintenance
Exogenous Factors	Stations Req'd	Overhead Labor
		Cost of Capital
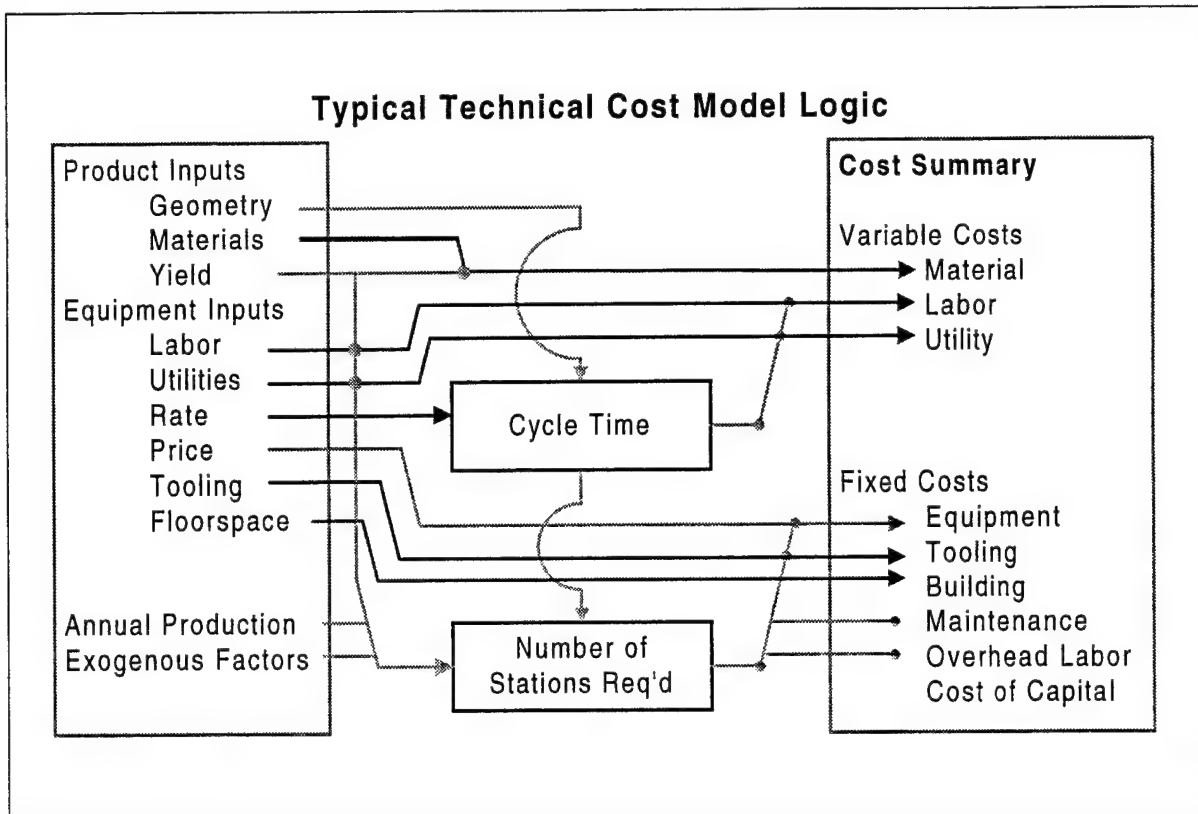
Figure 2. Foundation of Technical Cost Model

Predictive Relationships

The incorporation of predictive relationships, in the form of first-principles theory or equations that fit empirical data, allows the cost models to predict throughput rates, equipment prices, and other parameters as functions of input variables. Industry experts were consulted to provide modeling support ranging from overall strategy to the details of the deposition rate equations. The strategy aspect included the identification of input variables, definition of process conditions, and structure of the logic of the equations; while the detailed modeling included the actual equations, chemical reaction constants, and output trend verification.

Growth rates for CVD diamond are currently creating long cycle times that lead to high material, labor, and equipment costs due to low throughput per machine. However, industry data relating process parameters to growth rate are not readily available. For the modeling of commercial production a simplified deposition theory and its inherent assumptions has been incorporated into the Technical Cost Model in order to predict the scale-up costs of CVD diamond manufacture using the DC arcjet, microwave, and combustion flame technologies.

For the modeling of CVD diamond wafer manufacturing, the following intermediate outputs depend on inputs through predictive relationships:

- Deposition rate = f(reactor power, gas flow, gas mix, geometry)
- Equipment price = f(reactor power or deposition area)

The deposition rate relationship is established through first-principles diamond deposition theory, and the equipment price relationship is generated from industry data.

Implementing CVD Diamond Deposition Theory

The first-principles theory for CVD diamond deposition is contained as a module inside the CVD diamond TCMs. Inputs for the theories vary by technology. All three of the technologies in this report incorporate deposition theory.

DC Arcjet

Figure 3 is a diagram of the overall modeling strategy for the DC arcjet model, which is provided in Appendix A. The gas jet exiting the nozzle forms the first of two regimes; the chemistry in this region is a function of the reactor's input parameters and is assumed to be uniform. The second region is the boundary layer, where the chemistry varies with the distance from the growth surface. The goal of this approach is to calculate the atomic hydrogen concentration at the growth surface which, along with the CH_3 (methyl radical) concentration, determines the CVD diamond growth rate. Because of the interrelationships that exist among variables such as reactor power, gas concentrations, reactor pressure, gas

DC Arcjet Geometry Assumed For Simulations

Source: Goodwin, D.G., Memo to IBIS Associates, Inc., Jun. 1993.
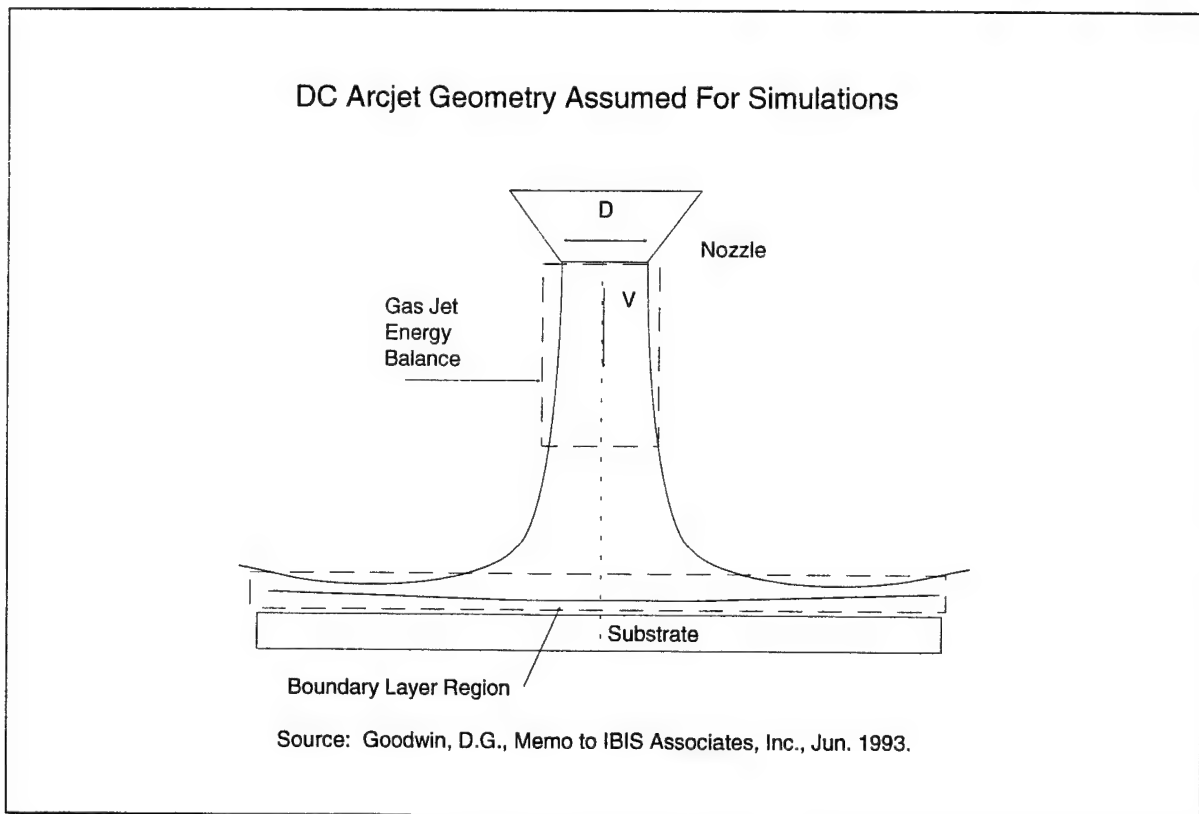
Figure 3. DC Arcjet Geometry

temperature, wafer diameter, and thermal conductivity, the calculation path to deposition rate is complex.

Figure 4 shows the logic flow for the deposition rate calculation in the DC arcjet model. Important calculations include the atomic hydrogen mole fraction in the gas jet (H Mole Frac. (Jet)), gas jet Mach Number (Mach Number), gas pressure at the substrate surface (Gas Pressure (Sub)), atomic hydrogen concentration at the substrate (H Concentr. (Sub)), and the linear deposition rate (Linear Dep. Rate).

IBIS DC Arcjet CVD Diamond Technical Cost Model Deposition Rate Equation

Legend

Inputs

Constants and Calculations
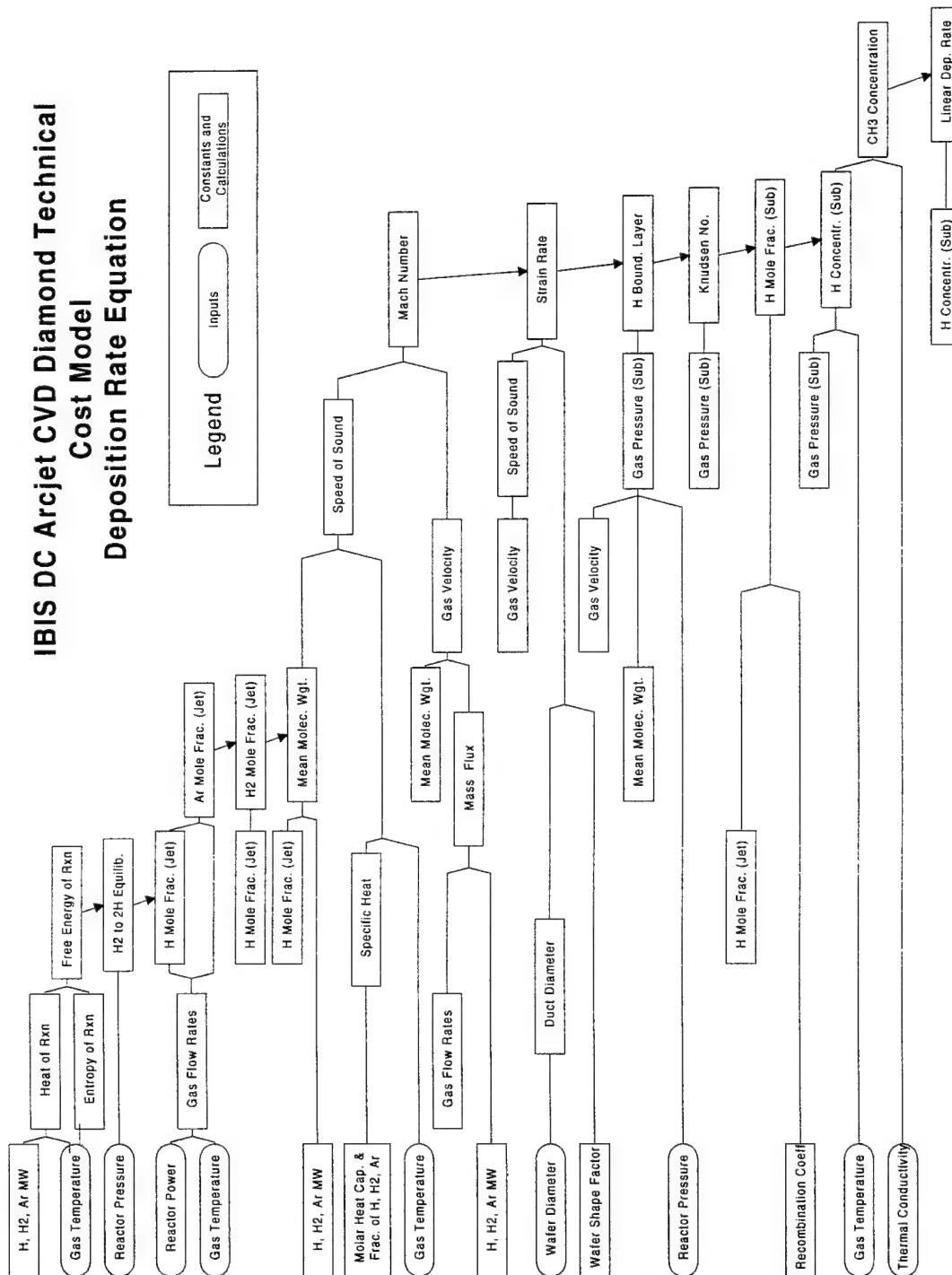
Figure 4. Logic Flow for DC Arcjet TCM

Microwave

Figure 5 is a diagram of the overall modeling strategy for the microwave model, which is provided in Appendix B. The model assumes atomic hydrogen is generated roughly in the middle of the plasma at a distance "L" from the substrate. The goal of this approach is to calculate the atomic hydrogen concentration at the growth surface through the characterization of both the diffusion of atomic hydrogen toward the surface and its recombination into H_2. Along with the CH_3 (methyl radical) concentration, the atomic hydrogen concentration at the surface determines the CVD diamond growth rate. Due to such variables as reactor power, reactor pressure, and thermal conductivity of the finished diamond, the calculation path to deposition rate is fairly complex.

Figure 6 shows the logic flow for the deposition rate calculation in the microwave model. Important calculations include the plasma ball diameter, atomic hydrogen generation rate (H Generation Rate), atomic hydrogen concentration at the substrate (H Concentr. @ Substrate), and the mass deposition rate.
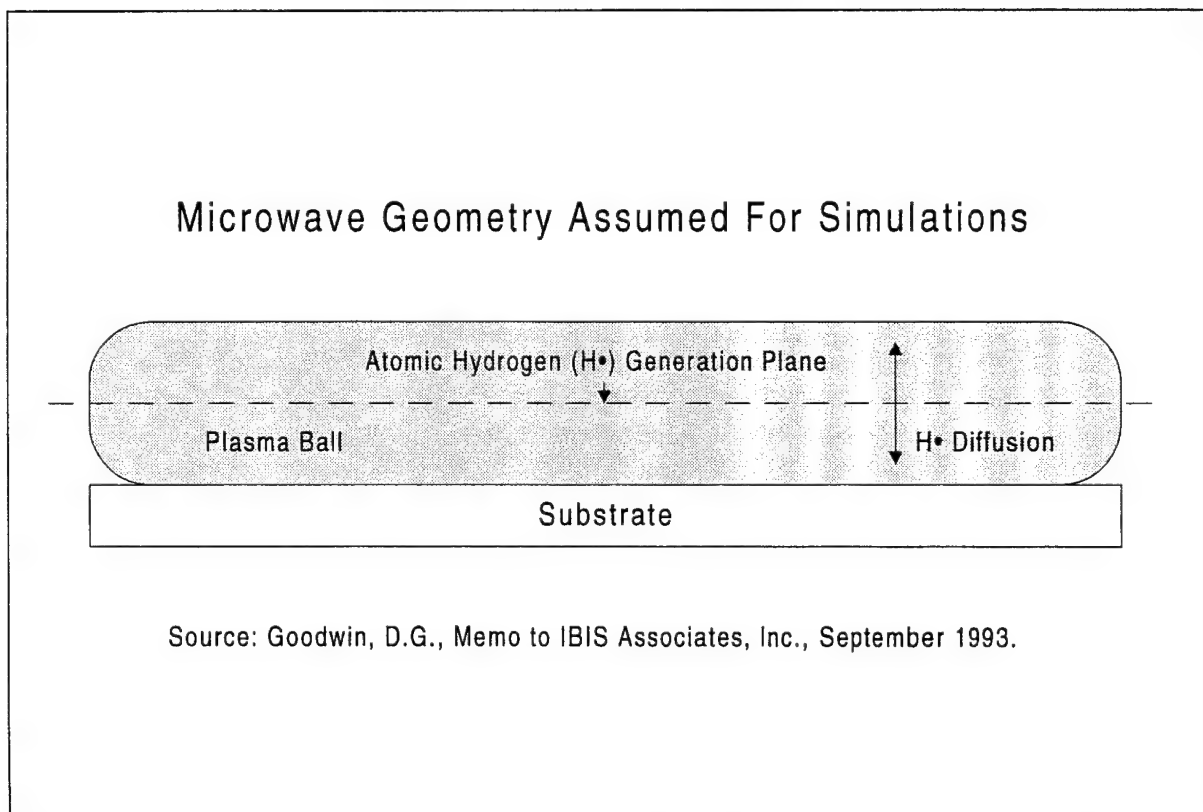
Figure 5. Microwave Geometry
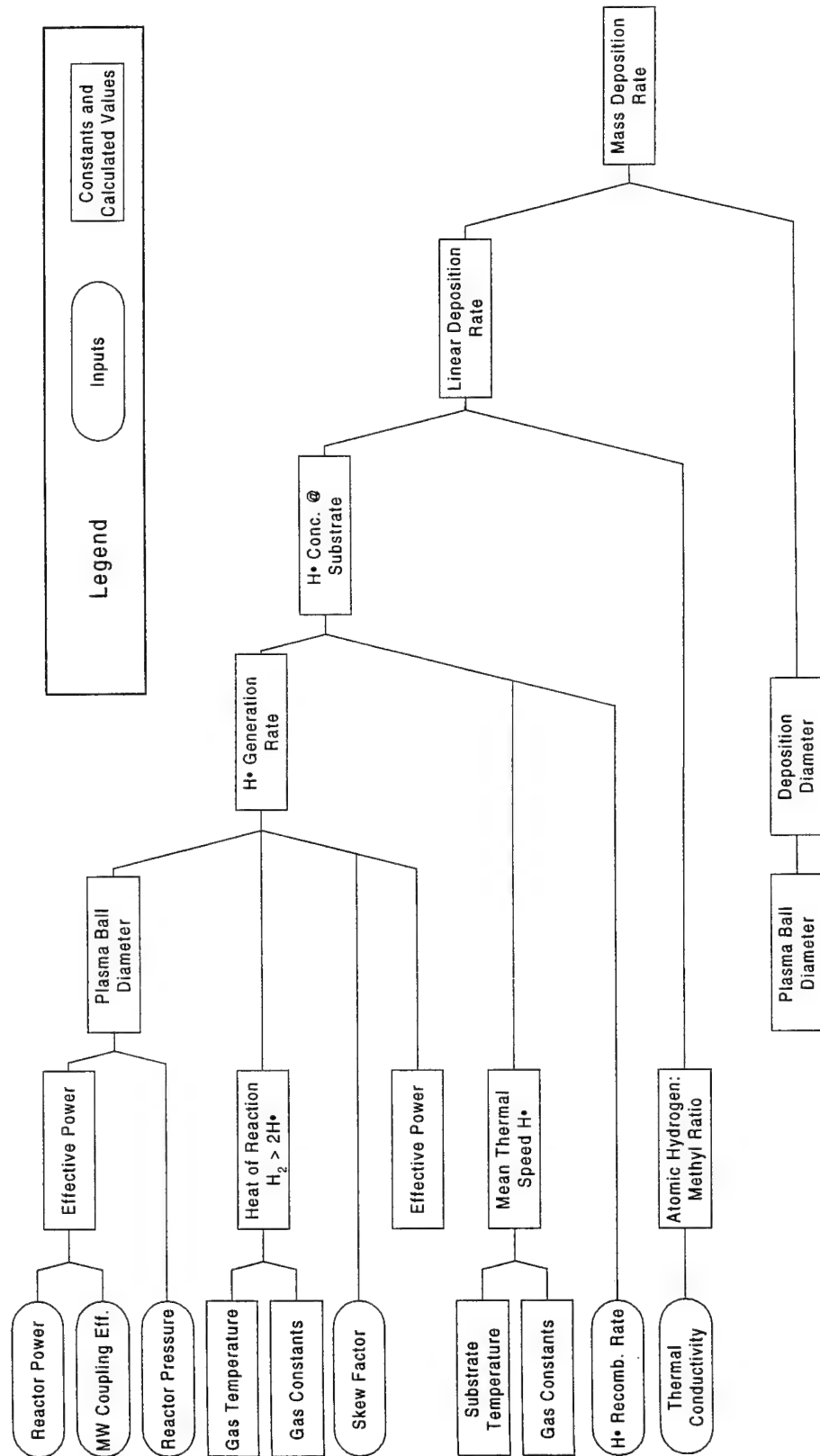
Figure 6. Logic Flow for Microwave TCM

Combustion Flame

Figure 7 is a diagram of the overall modeling strategy for the combustion flame model, which is provided in Appendix C. For numerical simulations that were generated by Professor Goodwin, it is assumed that the process gases are mixed and combust previous to accelerating through the nozzle. The resulting combustion jet is assumed to have uniform chemistry and velocity. Impinging on the substrate creates a boundary layer, through which atomic hydrogen and methyl radicals diffuse. The goal of this approach is to calculate the atomic hydrogen concentration at the growth surface which, along with the CH_3 (methyl radical) concentration, determines the CVD diamond growth rate. Due to such variables as gas concentration and thermal conductivity of the finished diamond, the calculation path to deposition rate is fairly complex.

Figure 8 shows the logic flow for the deposition rate calculation in the combustion flame model. Important calculations include the strain rate, atomic hydrogen concentration at the substrate, and the linear deposition rate.

For an explanation of the logic and actual equations that form the foundation of this deposition theory, see an article on this subject by Professor Goodwin (Goodwin, 1993).

Combustion Flame Geometry Assumed For Simulation
Single Nozzle, Attached Flame

Nozzle

D

V

L

Boundary Layer Region

Source: Goodwin, D.G., Memo to IBIS Associates, Inc., Dec. 1993.
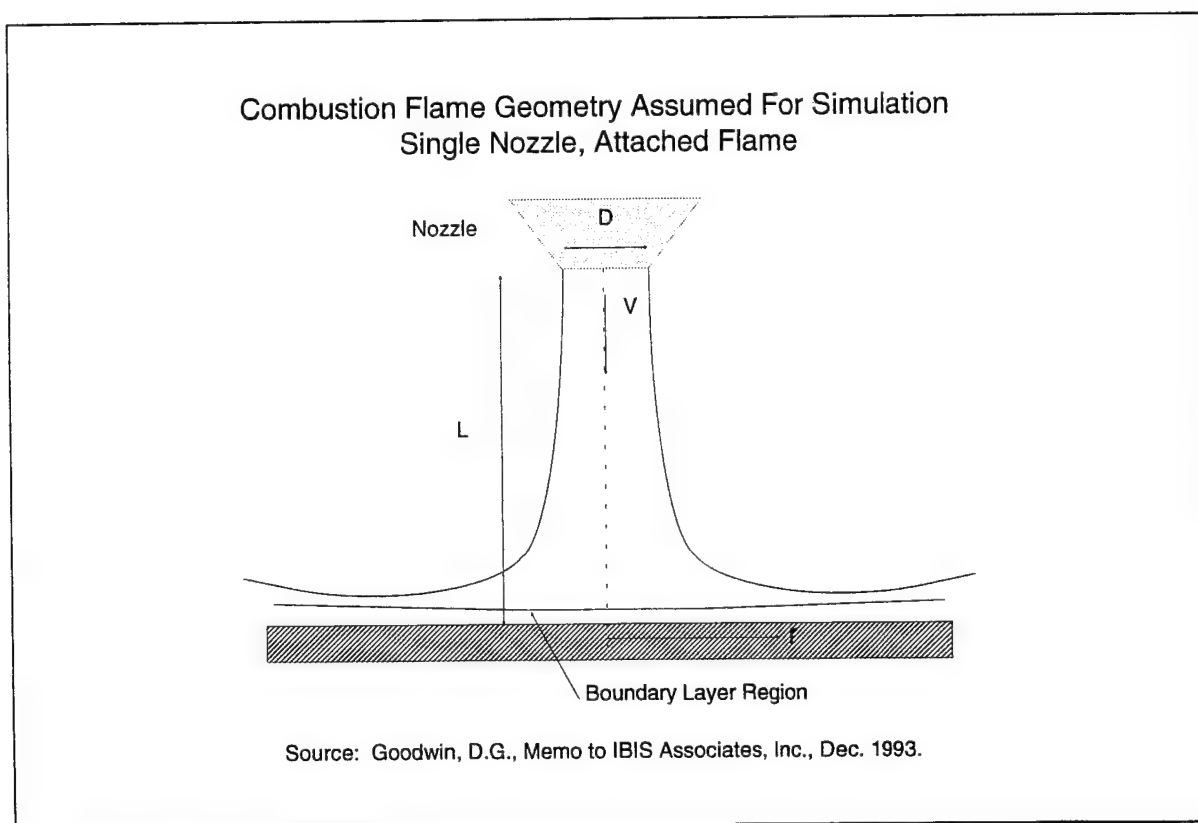
Figure 7. Combustion Flame Geometry

**IBIS Combustion Flame CVD Diamond
Technical Cost Model Deposition Rate Equation**
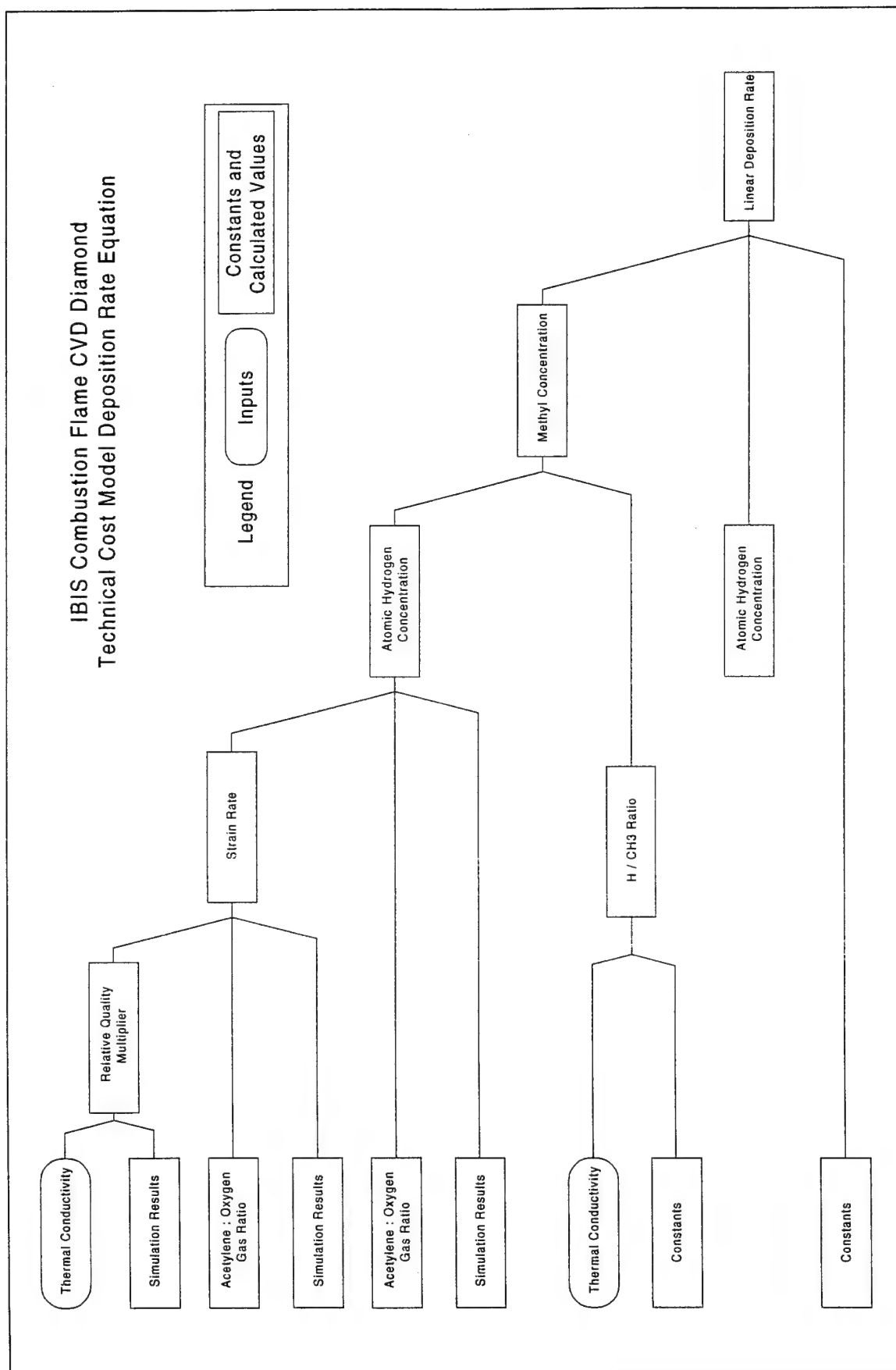
Figure 8. Logic Flow for Combustion Flame TCM

Exogenous Modeling Assumptions

For the modeling in this report, specific assumptions regarding the manufacturing operations and product specifications will be discussed in later sections. However, all of the cost models incorporate assumptions that relate to the time and place of manufacture. These inputs, such as labor wages and interest rates, are the same in all of the models and are shown in Table 2. Derived from the manufacturers in the US, these assumptions reflect an average manufacturing operation.

Table 2. Wage, Building Space, and Financial Assumptions

Exogenous Cost Factors		Units
Direct Wages	$13.33	/hr
Indirect Salary	$50,000	/yr
Indirect:Direct Labor Ratio	1.00	
Benefits on Wage and Salary	35%	
Working Days per Year	360	
Working Hours per Day	24	hrs
Capital Recovery Rate	10%	
Capital Recovery Period	5	yrs
Building Recovery Life	20	yrs
Working Capital Period	3	months
Price of Electricity	$0.050	/kWh
Price of Building Space	$100	/sqft
Price of Cooling Water	$0.03	/100 gal
Auxiliary Equipment Cost	15%	
Equipment Installation Cost	35%	
Maintenance Cost	8%	

Economics of CVD Diamond

This section shows results and sensitivities for the CVD diamond modeling scenarios. The following CVD diamond technologies are analyzed: DC arcjet, microwave, and combustion flame. The cost models for all three technologies include CVD diamond deposition theory, and the cost analysis related to these technologies focuses on the critical deposition parameters and cost sensitivities to these parameters.

Assumptions for the Long Term

While this report does provide cost model data for the three CVD diamond technologies, the underlying modeling assumptions should be understood before decisions or judgments are made. For instance, it is possible that a multiple nozzle setup for the combustion flame technology would be more efficient, and therefore cost less, than the single nozzle design assumed for this analysis. Given this potential, these results should be viewed as characterizing the costs of three specific technology implementations - not as representing three general technologies.

The significant assumptions for the CVD diamond cost models are presented in Table 3. This table reveals assumptions for the long term scenario for these technologies, where "long term" is defined as the expected state of diamond deposition five to ten years from today (i.e., in the years 2001 to 2006). With the assistance of industry experts, plausible product and process conditions have been selected to represent this long term scenario.

The long term power levels, deposition areas, and mass growth rates of the three technologies indicate their estimated progress. For the microwave technology, economies of scale are expected to be achieved using a power level of 200kW over a 20 inch diameter, depositing about six grams of diamond per hour. Compared to today, these assumptions reflect an increase in deposition area, which must be accompanied by a reactor power increase, and thereby results in a mass deposition rate increase. However, the linear growth rate is roughly the same as today's rates, since this technology is believed to be diffusion limited.

For the DC arcjet technology, the long term assumptions incorporate progress in reactor power, deposition area, and deposition rate. Higher reactor powers enable both larger deposition areas and higher gas jet temperatures, which boost the mass growth rate. These assumptions show the expected progress over the next five to ten years.

For the combustion flame technology, the deposition area is the only parameter to increase over current levels, due to the limited control of linear deposition rate and energy release (effective power) for this technology.

Table 3. Long Term Input Assumptions

	DC Arcjet	Microwave	Combustion
SELECTED INPUTS			
Wafer Thickness (microns)	500	500	500
Thermal Conductivity (W/mK)	1,000	1,000	1,000
Machine Power (kW)	125	200	108 (effective)
Deposition Yield (%)	90%	90%	90%
COMPUTED VALUES			
Wafer Diameter (cm)	30.5	51.1	8.9
Mass Deposition Rate (g/hr)	5.1	5.8	0.4
Linear Deposition Rate (um/hr)	20	8.0	17
Deposition Cycle Time (hrs)	25	63	30
Machine Cost ($/sta)	$500,000	$1,000,000	$125,000

Equipment cost also varies among the three technologies. The combustion flame technology has the lowest cost equipment, since the machine consists of only combustion-proof gas flow controls and equipment, a nozzle and nozzle cooling system, and waste gas removal system. The microwave technology possesses the highest cost equipment, due to the relatively higher cost of the power supply (versus DC arcjet), in addition to the vacuum system, radiation-leak-proof reactor, cooling system, and gas flow controls.

Unless stated otherwise, the values in Table 3 remain constant throughout the cost analyses in the following sections. Labor wages and other exogenous (accounting-related) cost factors are also held constant, and non-dedicated equipment is assumed (as if machines are rented - only the utilized percentage of annual equipment amortization is allocated to the product).

DC Arcjet

The DC arcjet technology is cost-sensitive to, among others, three process parameters: the reactor power, the upper limit on gas jet temperature (reactor limited), and the diameter of the diamond wafer being deposited. The gas flow rate is another significant process parameter affecting the cost of diamond but is an intermediate calculation based on the process variables above. The following sections provide insight into what can reduce the cost of CVD diamond produced by this technology.

Cost vs Reactor Power and Substrate Diameter

Figure 9 shows that, initially, deposition cost can be reduced by increasing the deposition diameter, but that increasing the power into the range of hundreds of kilowatts does not further reduce cost. The cost optimum is due to the sum of two effects: the cost initially

drops with larger areas, since the investment costs are being distributed over a greater mass; the cost then proceeds to rise as a result of a downward trend in growth rate, caused by the energy of the arcjet being distributed over higher deposition areas.

Figure 9 also indicates that there are diminishing returns on power increases. It does not, however, consider that there may be prohibitive engineering challenges when scaling up low powered reactors to high substrate diameters.

Cost vs Reactor Power and Gas Temperature

Figure 10 depicts the CVD diamond deposition cost as a function of both the reactor power and the temperature of the gas jet. The reigning transport theory suggests that a higher gas temperature allows more atomic hydrogen to reach the substrate, creating a higher growth rate which translates to lower cost. From interviews with industry experts, the upper limit on gas jet temperature is determined by the limitations of the DC arcjet torch nozzle. Therefore, Figure 10 indicates that the maximum allowable gas temperature must be determined in order to produce the lowest cost diamond. Fitting a curve to this data, the cost of diamond is inversely proportional to the gas temperature raised to the eighth power. This strong relationship means a gas temperature increase of just ten percent reduces the diamond cost by roughly fifty-three percent.

Cost Vs Reactor Power and Deposition Diameter

DC Arcjet Technology
Thermal Conductivity = 1,000 W/mK
Gas Temperature = 2,800 K
Thickness = 500 um

100 kW

200 kW

300 kW

Deposition Cost Per Carat

Substrate Diameter (cm)

Figure 9. DC Arcjet Results

Cost Vs Reactor Power and Jet Temperature

DC Arcjet Technology
Thermal Conductivity = 1,000 W/mK
Substrate Diameter = 6 inch
Thickness = 500 um
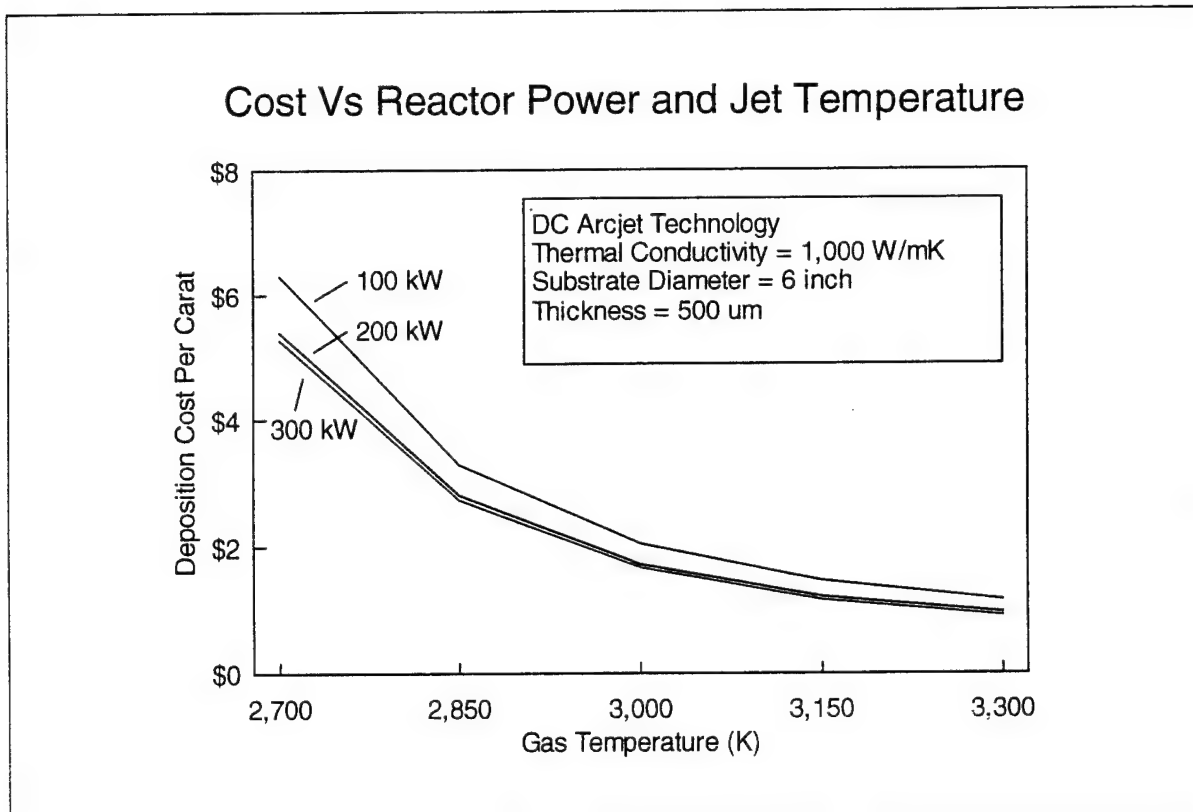
Figure 10. DC Arcjet Results

In contrast to the influence of gas jet temperature is the seemingly weak effect of reactor power on deposition cost. However, it should be noted that higher powered reactors would be necessary to produce higher gas temperatures.

The same warning given for the last sensitivity must be applied in this case: both high gas temperature and large substrates require higher power reactors, therefore the lower powered reactors may not be able to realistically attain the higher gas temperatures and diameters.

Microwave

The microwave technology is cost-sensitive to, among others, the reactor power. The reactor pressure and substrate diameter are other significant process parameters affecting the cost of diamond but are typically engineered to be optimized for each reactor power source. The following section provides insight into what can reduce the cost of CVD diamond produced by this technology.
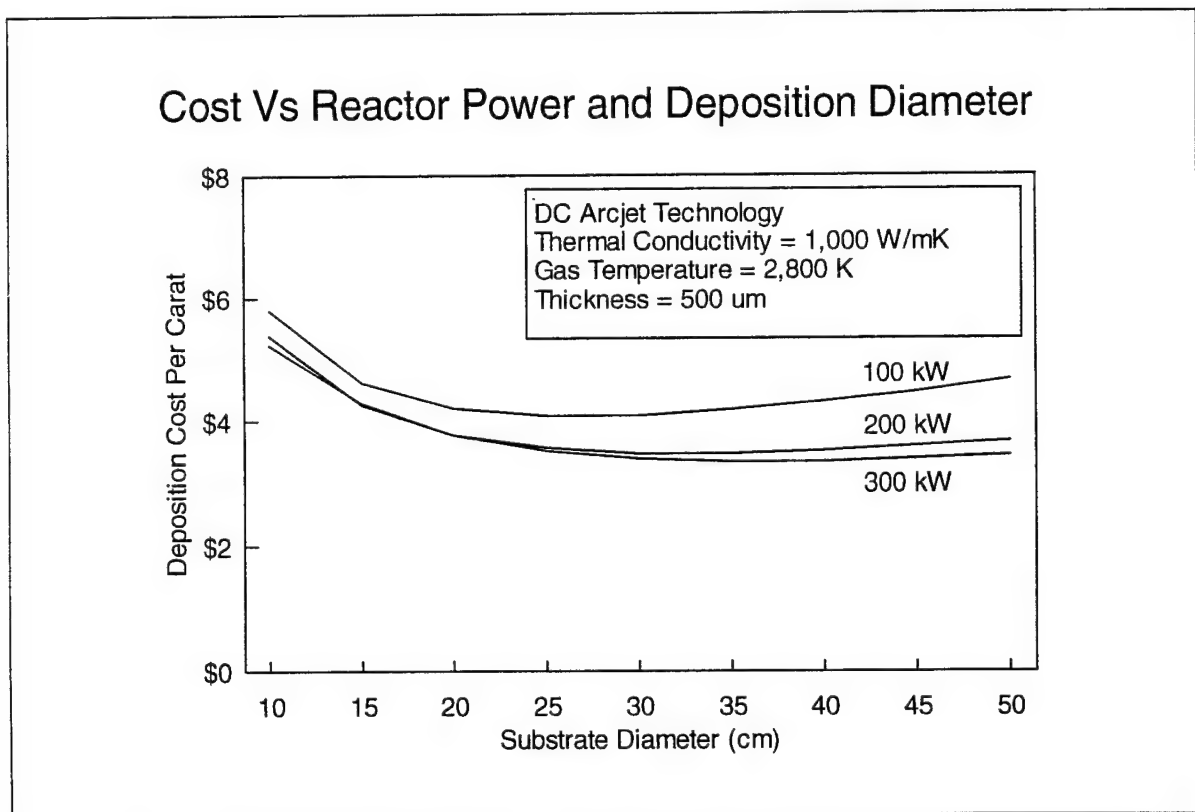
Cost vs Reactor Power

For this technology, process gases are excited into a plasma through microwave radiation. A plasma ball is formed in the reactor, its area proportional to the reactor power and inversely proportional to the reactor pressure. By increasing reactor power, therefore, this technology can be scaled to larger areas.

Figure 11 shows the cost per carat of CVD diamond as a function of reactor power. As noted in the figure, both reactor pressure and deposition diameter are dependents of reactor power. Fitting a curve to the data reveals that cost is inversely proportional to reactor power to the exponent 0.43, meaning a doubling of the power allows a twenty-five percent cost reduction. This sensitivity indicates that there are cost savings and possibly new applications for scaling up this technology to higher powers and areas.
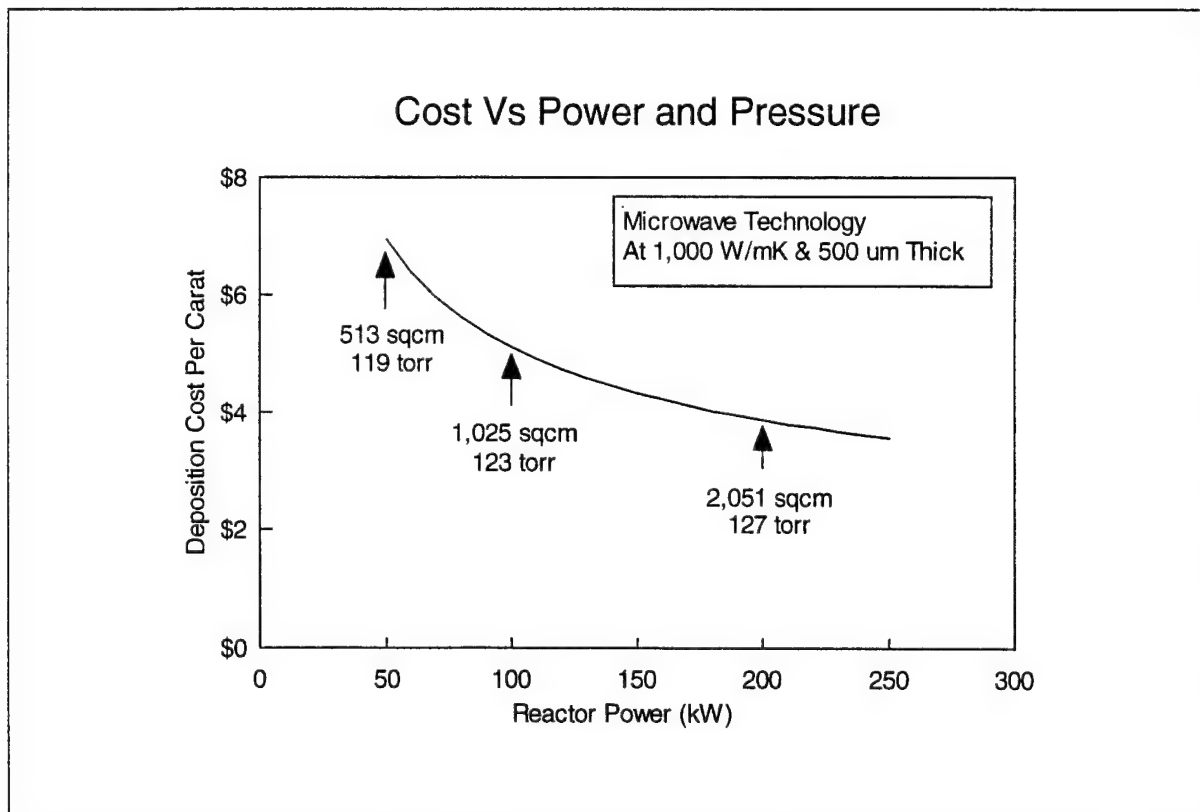
Figure 11. Microwave Results

Combustion Flame

The combustion flame technology is cost-sensitive to, among others, the following three parameters: the acetylene gas price, the ratio of acetylene to oxygen, and the substrate diameter. The gas flow rate is another significant process parameter affecting the cost of diamond but is dependent on the aforementioned input variables as well as the thermal conductivity target of the completed diamond film. If higher quality CVD diamond is desired, the gas flow rate must be increased, assuming the gas ratios are held constant. The following section provides insight into CVD diamond cost reduction through this technology.

Cost vs Acetylene:Oxygen Gas Ratio and Substrate Diameter

As shown in Figure 12, there is an optimal diameter for the combustion flame technology based on the single nozzle torch design assumed in the model. There exists an optimum due to the combination of two dynamics: one where increasing substrate diameter decreases the fixed costs (i.e., equipment investment) per carat, and the dynamic where gas costs vary with the cube of substrate diameter. Depending on the ratio of incoming acetylene to oxygen, the optimal substrate diameter ranges from ten centimeters at a gas ratio of 1.02 to six centimeters at a gas ratio of 1.10. The optimal substrate diameter varies inversely with thermal conductivity; at higher thermal conductivities the flow rates must also be higher to
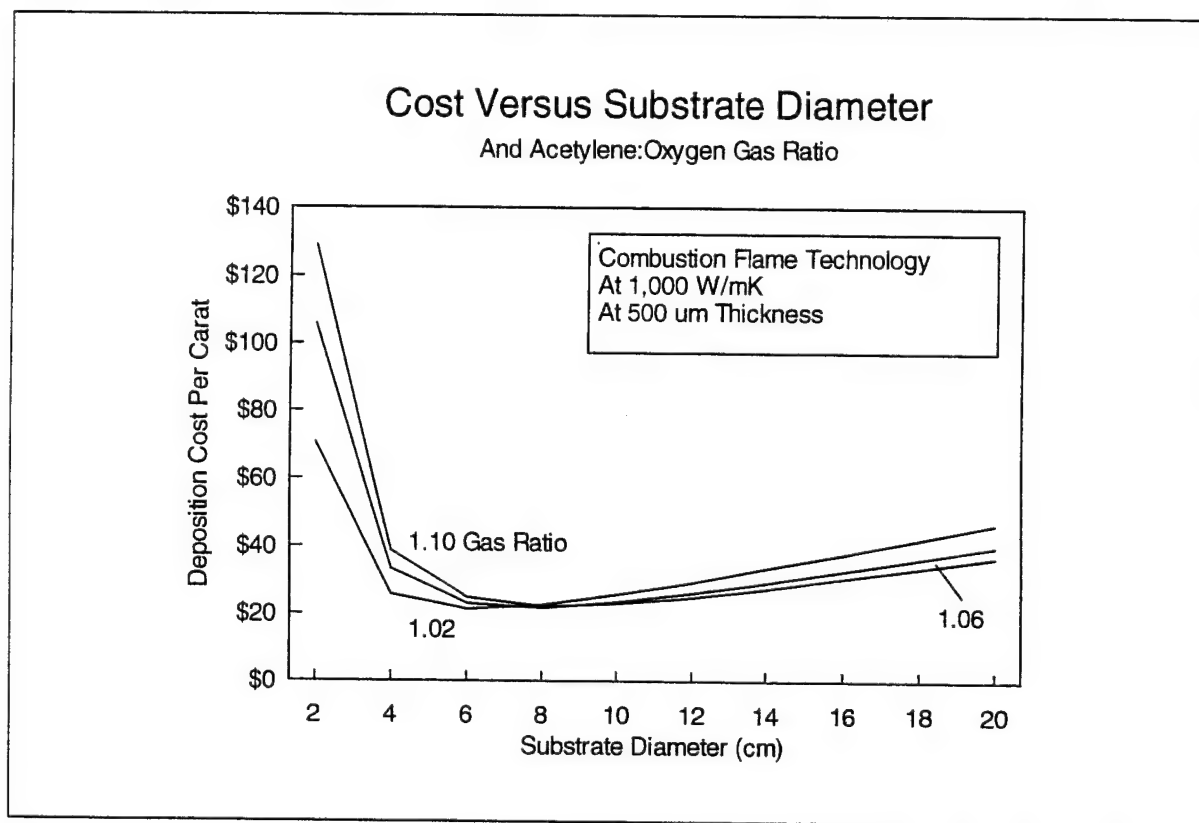
Figure 12. Combustion Flame Results

deliver more atomic hydrogen to the growth surface. With higher flow rates per unit mass of diamond produced, the material cost per carat increases.

Cost vs Acetylene Price

Expensive acetylene gas dominates the cost of combustion flame CVD diamond. Figure 13 reveals the cost sensitivity of this technology to acetylene pricing, in the event that acetylene production becomes more efficient over time. As reported previously, the long term pricing can drop to levels near the cost of generating acetylene gas: about $2.00 per standard cubic meter (SCM).

Even acetylene pricing as low as $0.50 per standard cubic meter cannot bring the cost per carat below the ten dollar level. This chart indicates that the single-nozzle combustion flame process as modeled for this report may not be the optimal for the combustion flame technology. Alternative nozzle geometries, cheaper process gases, or sub-atmospheric chamber pressures may boost the material utilization efficiency and therefore make this technology more competitive.
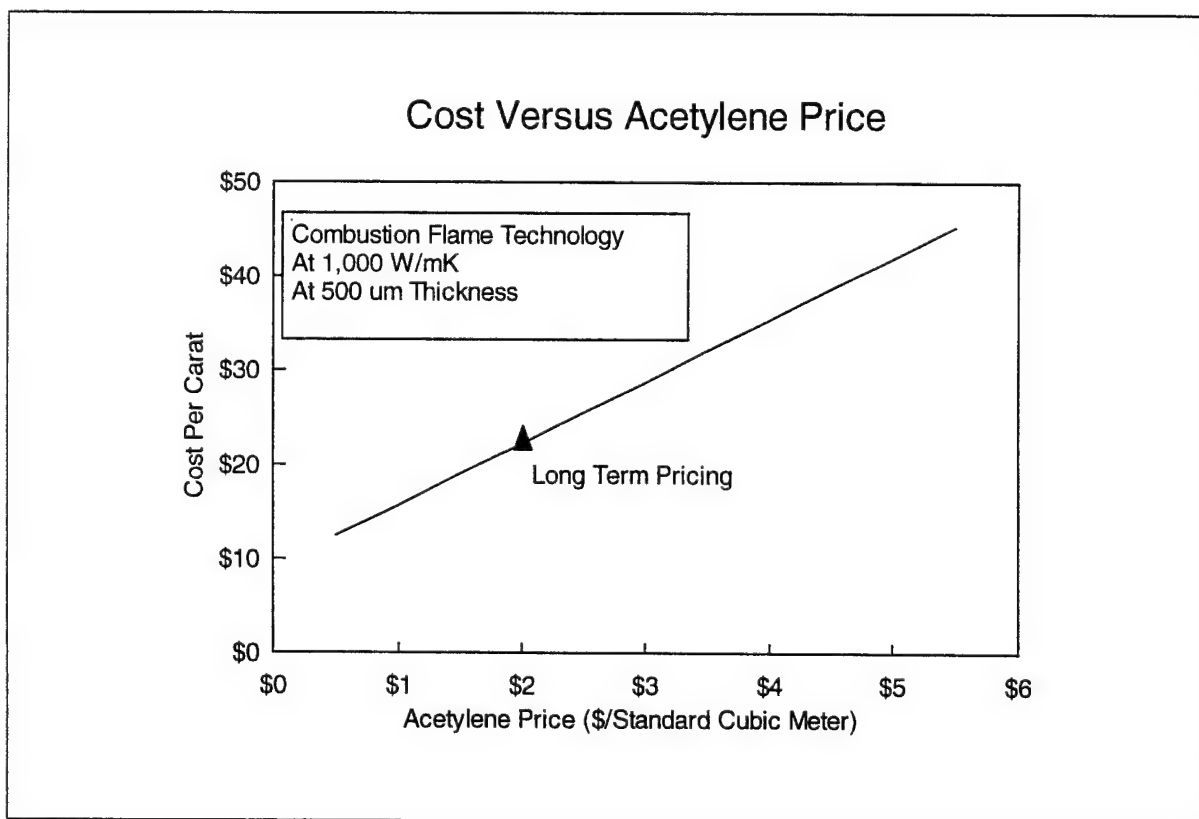
Figure 13. Combustion Flame Results

Technology Summary

Due to the rapid pace of technology development to date, this report's presentation of long term cost modeling should not be construed as a judgment of technologies. Instead, the results should be viewed as guidance for potential improvement in each individual technology.

Baseline Costs in the Long Term

Figure 14 shows the relative long term costs of the DC arcjet, microwave, and combustion flame technologies for the production of one-half millimeter thick CVD diamond wafers. The single nozzle combustion flame technology has the highest long term cost, at $22 per carat. The microwave and DC arcjet are significantly lower, at $3.87 and $3.76 per carat, respectively. The combustion flame technology is dominated by the material cost due to the high consumption rate of expensive process gases. The microwave technology has a significant equipment cost per carat due to the low growth rates and relatively high equipment price per machine. Lastly, the equipment cost is also significant for the DC arcjet technology, and its high consumption rate of process gases leads to a significant materials cost.

Implied in this analysis is that there will be demand in the long term for the quantities of CVD diamond produced by these deposition machines. For the DC arcjet technology, one
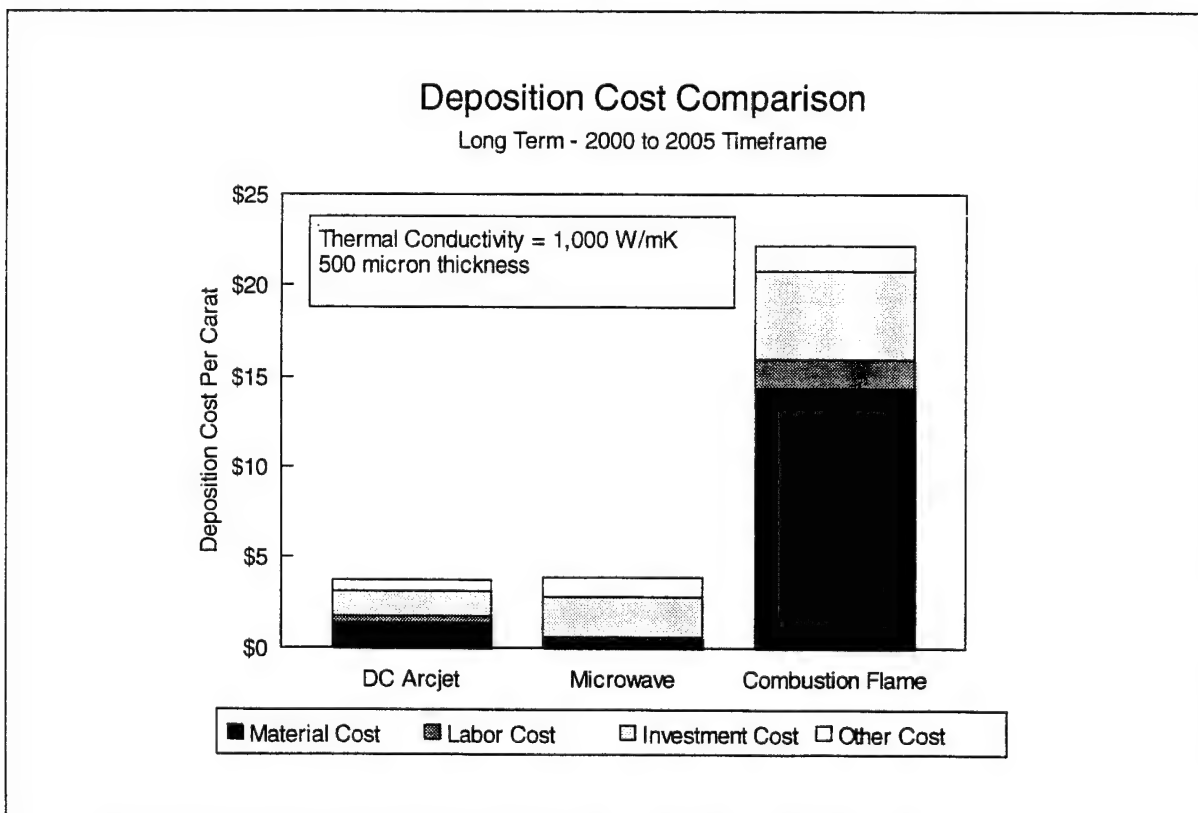
Figure 14. Three Technology Summary

machine will yield 167,000 carats per year, while the microwave reactor will yield 190,000 carats per year, and the combustion flame reactor will yield 11,000 carats per year.

Long Term Cost vs Thermal Conductivity

Competing materials for electronic thermal management applications range from as low as 200 W/mK (Aluminum) to as high as 800 W/mK (Copper/Carbon fiber composite). Industry experts believe the minimum thermal conductivity for CVD diamond would have to be higher than 800 W/mK in order to be competitive, depending on the selling price. Pure diamond has been measured at 2,000 W/mK, the upper limit for CVD diamond (although higher measurements have been made with synthetic diamond formed from pure C_{12}).

Thermal conductivity has been implemented as an input in the CVD diamond models. Figure 15 shows the cost per carat as a function of thermal conductivity for the these deposition models with long term input assumptions. In all cases, the cost of CVD diamond increases dramatically with thermal conductivity. In curve-fits to this data for the microwave and DC arcjet technologies, this exponent is 2.9 and 3.8 respectively. The combustion flame technology, while having the highest cost, has the lowest sensitivity to thermal conductivity with an exponent of 2.4. The impact of this result is more apparent with the following example: if the thermal conductivity requirements of a given application can be decreased by 10%, the CVD diamond cost will consequently decrease by 23% for
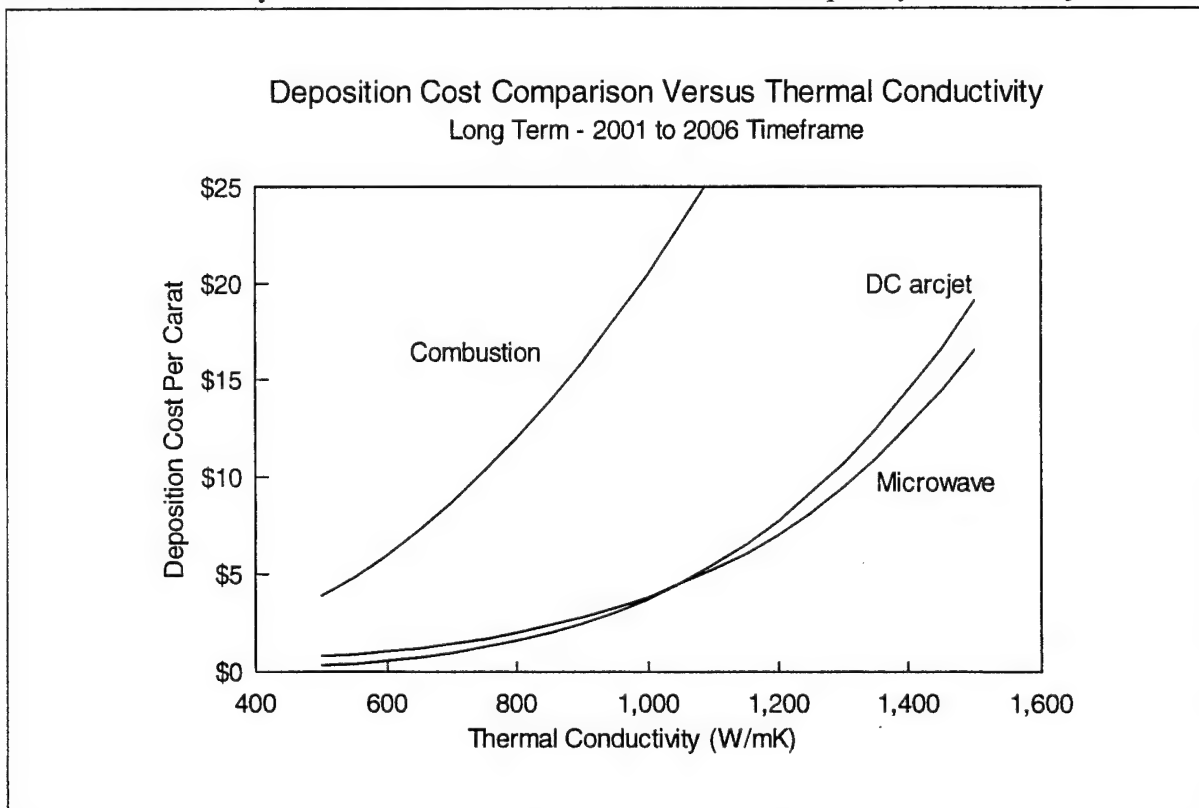
Figure 15. Three Technology Sensitivity

combustion flame diamond, 26% for microwave diamond, and 33% for DC arcjet diamond. Regardless of deposition technology, this analysis confirms that the desired thermal conductivity has a significant impact upon the cost of diamond: for a given application, the minimum acceptable value of thermal conductivity must be targeted before the CVD diamond is deposited.

CVD Diamond Cost Modeling Summary

Through the use of predictive equations in Technical Cost Models, the future (for the years 2001 to 2006) cost for CVD diamond at 1,000 W/mK is estimated in the $3 to $20 per carat range, depending on the deposition technology. With the TCM methodology predicting the cost as a function of various product and process parameters, sensitivities to critical inputs such as equipment power, gas prices, desired thermal conductivity, and deposition diameter have been analyzed.

Lowest Foreseeable CVD Diamond Cost

Appendix D contains a report by Professor David Goodwin of Caltech on the upper limits to diamond growth conditions. IBIS has implemented the logic and results of this report in order to estimate the lowest foreseeable cost of CVD diamond.

Using this analysis as a guide to the cost modeling, IBIS has investigated deposition conditions conducive to the upper limit of linear growth rate. As discussed in the appended analysis, the following parameters have theoretical limitations:

- Gas temperature = 5,000 K
- Stagnation point strain rate (a) = 10^5 s^{-1}
- Reactor pressure = 2,000 torr

Since gas temperature was revealed as the most important factor influencing the DC arcjet deposition rate in the previous analysis, the first step in determining the lowest foreseeable cost of CVD diamond was to set the model's maximum allowable gas jet temperature to 5,000 K.

However, in order to achieve this temperature in the gas at constant power, the flow rate of the process gases must be slowed, which then reduces the area of deposition. In order to maintain the deposition area, the velocity of the gas jet must remain at the same level as before, requiring a more powerful reactor to impart more energy to the gas.

Since the reactor power must increase to maintain the deposition area, an acceptable reactor power must be chosen for the 5,000 K gas jet temperature. However, as shown in Figure 9 for the DC arcjet analysis, each reactor power has an accompanying optimal deposition diameter. Figure 16 shows an analysis that optimizes the deposition diameter for a number of different reactor power settings, while maintaining the gas jet temperature at 5,000 K.

Figure 16 shows that DC arcjet CVD diamond cost reaches a minimum - $0.42 per carat - at the following conditions: a gas jet temperature of 5,000 K, a reactor arc power of 925 kW, and a deposition diameter of 110 cm (43 inches).

The factors contributing to the reduction of cost up to that optimum are the economies of scale with larger diameters and with higher powers. The factors contributing to the increase in cost after that optimum are the rising reactor price with power and the increasing gas usage with higher powers.

Table 4 lists significant input assumptions and outputs from the model for conditions leading to the lowest foreseeable cost. The gases, electricity, and equipment costs each constitute roughly one-third of the total cost. A 50% price reduction for any of these three
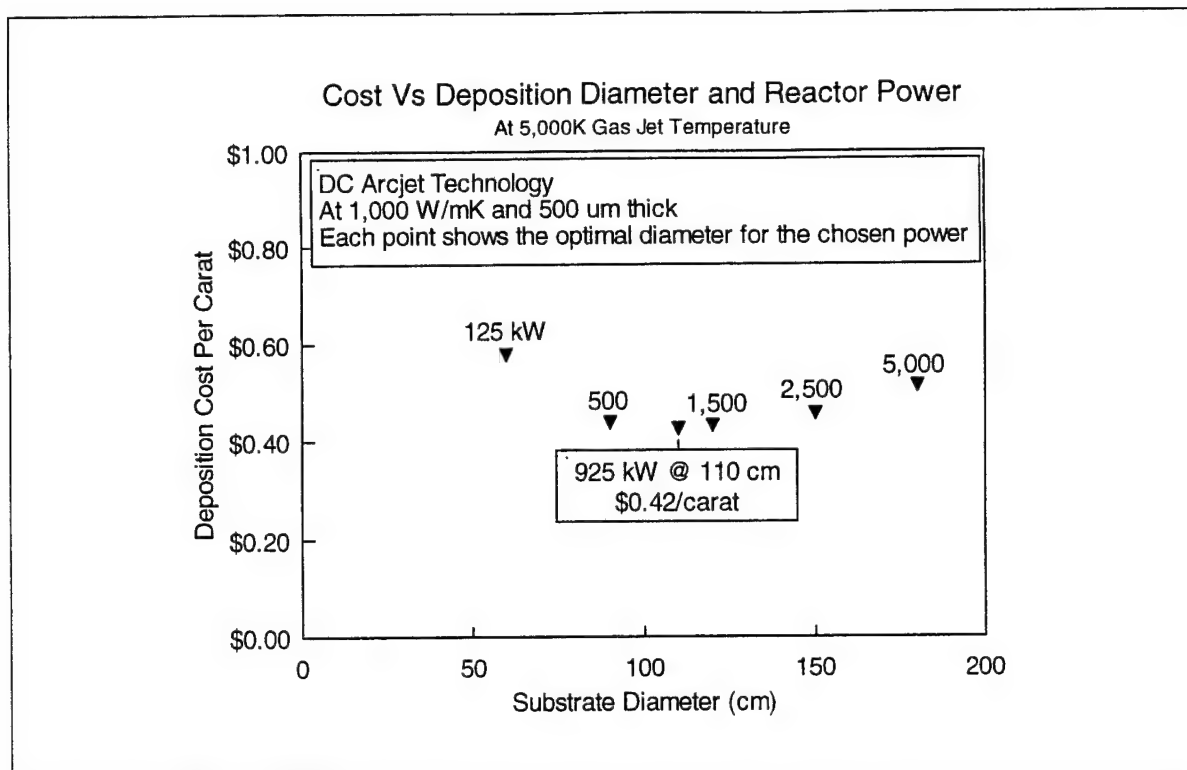
Figure 16. Lowest Foreseeable Cost Results

Table 4. CVD Diamond Modeling Input Assumptions

Selected Inputs and Outputs					
Product Specific Inputs			*Intermediate Outputs*		
Wafer Diameter	110	cm	Equipment Price	$942.000	/station
Finished Wafer Thickness	500	um	Gas Jet Velocity	5.772	cm/s
Thermal Conductivity	1,000	W/mK	Linear Deposition Rate	28.8	um/hr
			Mass Deposition Rate	96.1	g/hr
Process Related Inputs					
Power Imparted to Gas	925	kW	*Cost Summary Outputs*		
Gas Temperature	5,000	K	Material Cost (Gases)	$0.13	per carat
Reactor Pressure	50	torr	Labor Cost	$0.02	per carat
Hydrogen Gas Flow Rate	1,974	slm	Equipment Cost	$0.09	per carat
Methane Gas Flow Rate	20	slm	Electricity Cost	$0.11	per carat
Deposition Yield	90%		Other Cost	$0.08	per carat
			Total Cost	$0.42	per carat
Price Inputs					
Methane Price	$13.76	/SCM			
Hydrogen Price	$0.30	/SCM			
Price of Electricity	$0.050	/kWh			

factors (through gas pricing, electricity pricing, or equipment pricing) will reduce the CVD diamond deposition cost by 17%. The complete model is provided in Appendix E.

In summary, the IBIS DC Arcjet CVD Diamond TCM predicts the lowest foreseeable deposition cost at $0.42 per carat. Achieving this cost goal requires an arcjet deposition station costing $942,000 or less, electricity priced no higher than $0.05 per kWh, and hydrogen gas priced at or below $0.30 per standard cubic meter (SCM). Changes in these prices can cause the cost of CVD diamond to drop below the $0.42 per carat level. Additionally, this cost analysis assumes that the production of one machine - 3.1 million carats per year - will be absorbed by the market's demand for CVD diamond.

Survey Results

As part of the final report effort, IBIS Associates surveyed the US CVD diamond industry to solicit opinions on the future of CVD diamond deposition technologies. A copy of the questionnaire is provided in Appendix F.

Quantitative Responses

The responses had the following ranges of opinion for the following long term scenario parameters:

- Microwave technology
  - *Linear deposition rate - 8 um/hr to 22 um/hr*
  - *Overall yield (includes finishing) - 65% to 78%*
  - *All other assumptions were left unchanged*
- DC arcjet technology
  - *Linear deposition rate - 2.6 um/hr to 35 um/hr*
  - *Deposition Diameter - 30.5 cm to 92 cm*
  - *Overall yield (includes finishing) - 70% to 90%*
  - *Machine power - 125 kW to 375 kW*
  - *Machine cost per station - $400K to $1M*
  - *All other assumptions were left unchanged*
- Combustion flame technology
  - *Linear deposition rate - 30 um/hr to 40 um/hr*
  - *Overall yield (includes finishing) - 70% to 90%*
  - *Machine cost per station - $96K to $500K*
  - *All other assumptions were left unchanged*
- "Best case scenario" technology
  - *Machine cost*

    Low estimate - $100K to $600K

    Probable value - $150K to $1M

    High estimate - $200K to $1.5M
  - *Deposition yield*

    Low estimate - 70% to 80%

    Probable value - 80% to 90%

    High estimate - 90% to 95%
  - *Overall yield*

Low estimate - 60% to 75%

Probable value - 70% to 90%

High estimate - 85% to 95%

— *Deposition rate*

Low estimate - 0.33 um/hr to 10 um/hr

Probable value - 0.5 um/hr to 15 um/hr

High estimate - 1 um/hr to 30 um/hr

— *Machine power*

Low estimate - 15 kW to 100 kW

Probable value - 25 kW to 200 kW

High estimate - 30 kW to 300 kW

Selected Qualitative Responses

- Gas recycling

One response stressed the importance of recycling the process gases. While an option for gas recycle is incorporated in the DC arcjet TCM, IBIS chooses to assume that gases are not recycled for this technology based on the IBIS analysis of the economics of gas recycling.

- Combustion flame scaling

Regarding the combustion flame graph included with the survey, one response believed that the machine cost would scale more strongly with deposition diameter, making the cost rise after reaching an optimal deposition diameter. This effect has been included in the latest updates to the combustion flame TCM.

- Microwave gas mix

One source mentioned that the gas mix chosen for the microwave technology does not grow diamond. IBIS checked with microwave deposition experts and verified the microwave TCM.

- Overall yields

Many respondents believed that the overall yields would suffer with larger diamond diameters due to yield losses in finishing. However, IBIS assumes that the wafers can be diced prior to finishing so that high reliability sizes are used during finishing.

Overview of Previous Reporting

Appendix G provides the Executive Summaries from previous quarterly reports from this program (for only those quarters which contained reportable progress). These summaries review progress in modeling both CVD diamond deposition and diamond finishing, as well as side issues such as acetylene gas generation.

Additionally, IBIS has published papers relating to this research. These publications address the costs of deposition (Singer, 1994a) (Singer, 1994b) (Singer and Goodwin, 1995) (Singer and Busch, 1996 - to be published), the technology scale-up issues (Singer, 1994c), and planarization methods (Singer, 1994d).

Figure 1 showed progress for the US CVD diamond industry in reducing the costs of deposition. This one hundred-fold cost reduction is due to engineering advances resulting from increased understanding of CVD diamond deposition. However, a contributing factor to the deposition understanding, and therefore the cost reduction, has been industry's raised awareness to cost drivers as revealed by the IBIS Technical Cost Models developed as part of this program.

Summary

The extent of commercialization of man-made diamond depends on both the cost and performance of the product. The development efforts of many organizations have shown successful diamond manufacturing with respect to performance, but cost remains high for the film and coating versions of diamond.

Through the Technical Cost Modeling methodology, the paths to cost reduction have been identified for CVD diamond technologies. Economies of scale drives CVD diamond synthesis technologies: larger deposition areas and higher powers for the CVD method are required for further significant cost reduction.

Scaling up the deposition process reduces the cost of the CVD diamond technologies: the DC arcjet technology requires higher powers over optimal areas; the microwave method also should utilize larger areas and higher powers; and the combustion flame technology demands optimum areas with cheaper fuels. With CVD technologies, the long term (5-10 year timeframe) forecast suggests that costs on the order of $3 to $4 per carat are feasible.

The lowest foreseeable cost of CVD diamond has been identified through the identification of limiting factors in the deposition process. In this analysis, the lowest foreseeable cost for the DC arcjet technology is predicted at the $0.42 per carat level. Since such a diamond deposition machine would produce 3.1 million carats per year, it is assumed that a CVD diamond market of at least this size will exist. Further cost reduction can be achieved through obtaining lower-priced gases, electricity, and equipment than is assumed for this report.

In summary, the five to ten year outlook for CVD diamond entails lower cost. CVD diamond can be expected to drop by about two orders of magnitude as it completes the transition from research-size equipment to full manufacturing oriented equipment.

Acknowledgments

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Appendix A: The DC Arcjet Technical Cost Model

DC ARC-JET CVD DIAMOND TECHNICAL COST MODEL - LONG TERM

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Revision Date: 4/96

PRODUCT SPECIFICATIONS

Part Name	6 in. substrate		NAME
Wafer Diameter	30.48	cm	DIAM
Finished Wafer Thickness	500	um	THIK
Thermal Conductivity	1,000	W/mK	THERMCON
Annual Production Volume	1.0	(000/yr)	NUM
Length of Production Run	5	yrs	PLIFE

PROCESS RELATED FACTORS - DEPOSITION

Process In Use?	1	[1=Y 0=N]	USE2
Dedicated Investment	0	[1=Y 0=N]	DED2
Process Yield	90%		YLD2
Average Equipment Downtime	15%		DOWN2
Direct Laborers	0.40	/sta	NLAB2
Machine Power	125	kW	POW2
Power to Gas Efficiency	100%		P2GEFF
Machine Load/Unload Time	15	min/batch	PTIME2
Available Deposition Time	8,640	hrs/yr	DAYHR2
Coolant Temp. Rise	50	C	TEMP2
Heat Capacity of Coolant	1.0	cal/g/C	CP2
Building Space Requirement	1,500	sqft/sta	FLR2
Reactor Pressure	50	torr	RPRESS
Substrate Temperature	1,173	K	STEMP
Gas Temperature (>1000K)	2,800	K	GTEMP
Hydrogen Gas Flow Rate	1,096.5	slm	HFLOW
Carbon Fas Flow Rate	11.0	slm	CFLOW
Argon Gas Flow Rate	0.0	slm	ARFLOW
Other Gas Flow Rate	0.0	slm	OGFLOW

Total Gas Flow Rate	1,107.4	slm	

	Menu #	vol%	
Hydrogen	3	99.0%	GASA VOLA
Carbon Containing Gas	16	1.0%	GASB VOLB

Carrier Gas	0	0.0%	GASC VOLC
Other Gas	0	0.0%	GASD VOLD
		100.0%	

Hydrogen Recycle Rate	0%	RECYC
Carrier Gas Recycle Rate	0%	RECYC2
Gas Recycle Equipment Cost	$250,000 total	MCH2A

Recombine Coef. (gammaH)	0.10	RECOMBX
Substrate:Duct Area Ratio	3.00	SUBDUCT
Substrate Shape Factor (c)	1.00	SHAPFAC
Diamond Density	3.51 g/cc	DENS
Ideal Gas Constant (R)	62,358 cc torr/K mol	IDEALG1
Ideal Gas Constant 2 (R)	8.31 J / mol K	IDEALG2

NASA Enthalpy Constants	H2	H	Ar
a1	2.99E+00	2.50E+00	2.50E+00
a2	7.00E-04	0.00E+00	0.00E+00
a3	-5.63E-08	0.00E+00	0.00E+00
a4	-9.23E-12	0.00E+00	0.00E+00
a5	1.58E-15	0.00E+00	0.00E+00
a6	-8.35E+02	2.55E+04	-7.45E+02
a7	-1.36	-0.46	4.37
MW	2.02	1.01	39.95

EXOGENOUS COST FACTORS

Direct Wages	$13.33 /hr	WAGE
Indirect Salary	$50,000 /yr	SALARY
Indirect:Direct Labor Ratio	0.50	ILAB
Benefits on Wage and Salary	35%	BENI
Working Days per Year	360	DAYS
Working Hours per Day	24 hr	HRS
Capital Recovery Rate	10%	CRR
Capital Recovery Period	5 yrs	ELIFE
Building Recovery Life	20 yrs	BLIFE
Working Capital Period	3 months	WCP
Price of Electricity	$0.050 /kWh	ELEC
Price of Natural Gas	$6.50 /MBTU	GAS
Price of Building Space	$100 /sqft	PBLD
Price of Cooling Water	$0.03 /100 gal	WATER
Auxiliary Equipment Cost	15%	AUX
Equipment Installation Cost	35%	INST
Maintenance Cost	8%	MNT

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    DC ARC CVD TCM:              DEPOSITION

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	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$853.38	$853,384	35.5%	
Direct Labor Cost	$237.65	$237,647	9.9%	
Utility Cost	$178.34	$178,342	7.4%	
FIXED COST ELEMENTS				
Equipment Cost	$573.03	$573,030	23.8%	$3,000,000
Tooling Cost	$0.00	$0	0.0%	$0
Building Cost	$28.65	$28,652	1.2%	$600,000
Maintenance Cost	$275.05	$275,054	11.4%	
Overhead Labor Cost	$38.20	$38,202	1.6%	
Cost of Capital	$221.64	$221,639	9.2%	
TOTAL FABRICATION COST	$2,405.95	$2,405,950	100.0%	$3,600,000

INTERMEDIATE CALCULATIONS

Process In Use	1.00 [1=Y 0=N]	PRO2
Cumulative Yield	90.0%	CYLD2
Effective Production Volume	1,111 /yr	ENUM2

ENERGY BALANCE CALCULATIONS

	H_2	H	Ar	
Enthalpy Per Unit Mass	40,361	267,863	1,302	J/g
Molar Enthalpy	81,360	269,979	52,003	J/mol
Molar Entropy	200.25	161.16	201.28	J/K mol
Molar Heat Capacity (Cp)	36.62	20.79	20.79	J/K mol

Heat of Reaction ($H_2 ==> 2H$)	458,597	J/mol
Entropy of Rxn ($H_2 ==> 2H$)	122	J/K mol
Free Energy of Rxn ($H_2 ==> 2H$)	116,809	J/mol
Equilibr Const Kp ($H_2 ==> 2H$)	6.62E-03	

Mole Fraction H	27.09%
Mole Fraction Argon	0.00%
Mole Fraction H_2	72.91%
Total Molar Enthalpy	132,453 J/mole

Mean Molecular Weight	1.74 g/mole	
Mean Specific Enthalpy	76,001 J/g	
Mean Molar Heat Capacity	32.33 J/K mol	
Deposition Arc Power	125 kW	DAPOW2
Duct Area (A inf.)	243.22 sqcm	DCTAREA
Duct Diameter	17.60	DCTDIAM
Mass Flux	1.64 g/s	
Gas Velocity (U inf.)	13,548 cm/s	
Specific Heat Ratio (gamma)	1.35	
Speed of Sound	424,055 cm/s	
Mach Number	0.03	

Note: Adjust Input Temperature (cell B47) such that Temp. Solver = 0

Input Temperature	2,800 K	
Temperature Solver	-1.46E-11	

BOUNDARY LAYER CALCULATIONS

Strain Rate (a)	770 1/s	
Gas Pressure at Substrate	50.03 torr	
Hydrogen Boundary Layer	0.82 cm	
Thermal Boundary Layer	0.71 cm	
H Mean Free Path (lambda)	2.80E-03 cm	
Knudsen Number	3.43E-03	
H Mole Fraction at Substrate	0.90%	
H Concentration at Substrate	6.15E-09 mol/cc	
H/CH3 Ratio	10.89	
CH3 Concentration at Substr.	5.65E-10 mol/cc	

DEPOSITION RATE CALCULATIONS

Mass of Diamond Deposited	128.06 g	MASS2
Linear Deposition Rate	20.0 um/hr	LINDEP2
Mass Deposition Rate	5.1 g/hr	MASDEP2
Deposition Time	25.00 hrs	CTIMEB2
Machine Setup Time	0.25 hrs	CTIMEA2
Single Machine Productivity	290 wafers/year	SMPR2
Runtime for One Station	382%	RTIME2
Number of Parallel Stations	3.82	NSTAT2
Total Hydrogen Gas Volume	1644.69 SCM	HGAS2

	Consumption (SCM/pc)	Cost ($/pc)		
Total Argon Gas Volume	0.00 SCM		ARGAS2	
Total Carbon Gas Volume	16.45 SCM		CARGAS2	
Total Gas Volume	1,661 SCM		TVOL2	
Total Gas Flow Rate	1,107,423 sccm		FLOWR2	
Carbon Capture Factor	1.59%		CCF2	

	Consumption (SCM/pc)	Cost ($/pc)		
Hydrogen Consumption	1644.69	$493.41	GASA2	COSTA2
Carbon Gas Consumption	16.45	$226.31	GASB2	COSTB2
Carrier Gas Consumption	0.00	$0.00	GASC2	COSTC2
Other Gas Consumption	0.00	$0.00	GASD2	COSTD2
Energy Requirement	3,125 kWh/pc		ENERGY2	
Cooling Water Flow Rate	9.5 gal/min		WATER2	
Cooling Water Requirement	14,194 gal/pc		COOL2	
Building Space/Station	1,500 sqft		SPACE2	
Recycle Equipment Cost	$0 /sta		REC2	
Liquid Hydrogen Tank Rental	$4,475 /mo/tank		HYD2	
Liq Carrier Gas Tank Rental	$0 /mo/tank		CAR2	
Gas Storage Equipment Rent	$53,700 /year		GTANK2	
Machine Cost	$500,000 /sta		MCH2B	
Installed Equipment Cost	$675,000 /sta		IEQUIP2	
Auxiliary Equipment Cost	$75,000 /sta		AEQUIP2	
Equipment Annuity	$730,512 /yr		EINT2	
Tooling Annuity	$0 /yr		TINT2	
Building Annuity	$66,358 /yr		BINT2	
Working Annuity	$1,609,080 /yr		WINT2	

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    DC ARC CVD TCM:            COST SUMMARY

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	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$853.38	$853,384	35.5%	
Direct Labor Cost	$237.65	$237,647	9.9%	
Utility Cost	$178.34	$178,342	7.4%	
FIXED COST ELEMENTS				
Equipment Cost	$573.03	$573,030	23.8%	$3,000,000
Tooling Cost	$0.00	$0	0.0%	$0
Building Cost	$28.65	$28,652	1.2%	$600,000
Maintenance Cost	$275.05	$275,054	11.4%	
Overhead Labor Cost	$38.20	$38,202	1.6%	
Cost of Capital	$221.64	$221,639	9.2%	
TOTAL FABRICATION COST	$2,405.95	$2,405,950	100.0%	$3,600,000

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SUMMARY INFORMATION

Part Name	6 in. substrate	
Total Direct Laborers	6.60	/shift
Total Floor Space	7,350	sqft
Total Capital Investment	$3.6	MM
Area Cost	$3.30	/sqcm
Cost Per Carat	$3.76	/ct
Number of Carats Per Wafer	640.28	carats/wafer
Machine Throughput	167,112	ct/year/mch

Appendix B: The Microwave Technical Cost Model

MICROWAVE CVD DIAMOND TECHNICAL COST MODEL
IBIS ASSOCIATES, INC.   Copyright (c) 1996 v4.0

Revision Date: 4/96

PRODUCT SPECIFICATIONS

Part Name	20 in. substrate		NAME
Finished Wafer Thickness	500	um	THIK
Thermal Conductivity	1,000	W/mK	THERMCON
Annual Production Volume	1	(000/yr)	NUM
Length of Production Run	5	yrs	PLIFE

PROCESS RELATED FACTORS - DEPOSITION

Process In Use?	1.00	[1=Y 0=N]	USE2	
Dedicated Investment	0.00	[1=Y 0=N]	DED2	
Process Yield	90.0%		YLD2	
Average Equipment Downtime	15.0%		DOWN2	
Direct Laborers	0.10	/sta	NLAB2	
Rated Microwave Power	200	kW	POW2	>5 kW
Reactor Pressure	127.4	torr	PRES2	
Plasma Area Utilization	200%		DAU2	
Recombine Coef. (gammaH)	0.10		HRECOMB2	
Plasma Ball Skew Factor (f)	3.00	(2=sym.)	SKEW2	
Diamond Density	3.51	g/cc	DENS	
Ideal Gas Constant (R)	62,358	cc torr/K mol	IDLGAS2A	
Ideal Gas Constant 2 (R)	8.31	J / mol K	IDLGAS2B	

NASA Enthalpy Constants	H_2	H		
a1	2.99E+00	2.50E+00	H2EN2A	HEN2A
a2	7.00E-04	0.00E+00	H2EN2B	HEN2B
a3	-5.63E-08	0.00E+00	H2EN2C	HEN2C
a4	-9.23E-12	0.00E+00	H2EN2D	HEN2D
a5	1.58E-15	0.00E+00	H2EN2E	HEN2E
a6	-8.35E+02	2.55E+04	H2EN2F	HEN2F
a7	-1.36	-0.46	H2EN2G	HEN2G
MW	2.02	1.01	H2MW	HMW

	Menu #	vol%		
Hydrogen	9	89.0%	GASA	VOLA
Carbon Containing Gas	16	10.0%	GASB	VOLB
Carrier Gas	0	0.0%	GASC	VOLC
Other Gas	25	1.0%	GASD	VOLD

Hydrogen Recycle Rate	0.0%	RECYC
Carrier Gas Recycle Rate	0.0%	RECYC2
Gas Recycle Equipment Cost	$250,000 total	MCH2A
Microwave Coupling Eff.	98%	P2GEFF2
Total Power Multiplier	120%	TPM2
Carbon Capture Factor	10.0%	CCF2
Machine Load/Unload Time	15.00 min/batch	PTIME2
Available Deposition Time	8,640 hrs/yr	DAYHR2
Microwave Tube Life	10000 hrs	LIFE2
Coolant Temp. Rise	7.00 C	TEMP2
Heat Capacity of Coolant	1.0 cal/g/C	CP2
Building Space Requirement	400 sqft/sta	FLR2

EXOGENOUS COST FACTORS

Direct Wages	$13.33 /hr	WAGE
Indirect Salary	$50,000 /yr	SALARY
Indirect:Direct Labor Ratio	0.50	ILAB
Benefits on Wage and Salary	35.0%	BENI
Working Days per Year	360.00	DAYS
Working Hours per Day (*)	24.00 hr	HRS
Capital Recovery Rate	10%	CRR
Capital Recovery Period	5.00 yrs	ELIFE
Building Recovery Life	20.00 yrs	BLIFE
Working Capital Period	3.00 months	WCP
Price of Electricity	$0.050 /kWh	ELEC
Price of Natural Gas	$6.50 /MBTU	GAS
Price of Building Space	$100 /sqft	PBLD
Price of Cooling Water	$0.03 /100 gal	WATER
Auxiliary Equipment Cost	15.0%	AUX
Equipment Installation Cost	35.0%	INST
Maintenance Cost	8.0%	MNT

	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$859.17	$859,165	12.3%	
Direct Labor Cost	$147.65	$147,653	2.1%	
Utility Cost	$951.88	$951,885	13.7%	
FIXED COST ELEMENTS				
Equipment Cost	$2,849.13	$2,849,127	40.9%	$15,004,630
Tooling Cost	$60.00	$60,000	0.9%	$300,000
Building Cost	$18.99	$18,988	0.3%	$400,000
Maintenance Cost	$1,170.03	$1,170,032	16.8%	
Overhead Labor Cost	$23.74	$23,735	0.3%	
Cost of Capital	$877.17	$877,170	12.6%	
TOTAL FABRICATION COST	$6,957.76	$6,957,755	100.0%	$15,704,630

INTERMEDIATE CALCULATIONS

Process In Use	1.00	[1=Y 0=N]	PRO2
Cumulative Yield	90.0%		CYLD2
Effective Production Volume	1,111 /yr		ENUM2
Delivered Power	196.0 kW		EPOW2

HYDROGEN DIFFUSION CALCULATIONS

	H2	H·	
Enthalpy Per Unit Mass	385	271,987	J/g
Molar Enthalpy	776	274,136	J/mol
Molar Entropy	202.79	162.59	J/K mol
Molar Heat Capacity (Cp)	37.11	20.79	J/K mol
Heat of Reaction (H2==>2H·)	547,496 J/mol		HTRXN2
Plasma Ball Diameter	36.13 cm		BDIAM2
Plasma Ball Area	2050.53 sq cm		BAREA2
Deposition Diameter	51.10 cm		DDIAM2
Mean H· Thermal Speed	502,063 cm/s		HSPEED2
H· Generation Rate	5.82E-05 mol/s/cc		HGEN2
H· Conc. at Substrate	9.27E-10 mol/cc		HCONC2
H/CH3 Ratio	10.89		HCH3R
CH3 Concentration	8.52E-11 mol/cc		CH3CON2

DEPOSITION RATE CALCULATIONS

Mass of Diamond Deposited	359.87 g		MASS2
Linear Deposition Rate	8.0 um/hr		LINDEP2
Mass Deposition Rate	5.8 g/hr		MASDEP2
Deposition Time	62.50 hrs		CTIMEB2
Machine Setup Time	0.25 hrs		CTIMEA2
Single Machine Productivity	117 wafers/year		SMPR2
Runtime for One Station	949%		RTIME2
Number of Parallel Stations	9.49		NSTAT2
Total Carbon Gas Volume	7.33 SCM		CARGAS2
Total Gas Volume	73 SCM		TVOL2
Total Gas Flow Rate	19,553 sccm		FLOWR2

	Consumption (SCM/pc)	Cost ($/pc)		
Hydrogen Consumption	65.26	$745.43	GASA2	COSTA2
Carbon Gas Consumption	7.33	$112.11	GASB2	COSTB2
Carrier Gas Consumption	0.00	$0.00	GASC2	COSTC2
Other Gas Consumption	0.73	$1.63	GASD2	COSTD2

Energy Requirement	14,701 kWh/pc	ENERGY2
Physical Tube Life	1.36 years	TLIFE2
Number of Tubes per Station	4 incl. orig.	NTUBE2
Number of New Tubes /Sta	0 /sta	NTUBE2A
Number of Refurb /Sta	3 /sta	NTUBE2B
New Microwave Tube Cost	$20,000 /tube	TUBE2A
Reworked Microwave Tube Cost	$10,000 /tube	TUBE2B
Cooling Water Flow Rate	108.1 gal/min	WATER2
Cooling Water Requirement	405,553 gal/pc	COOL2
Building Space/Station	400 sqft	SPACE2
Recycle Equipment Cost	$0 /sta	REC2
Liquid Hydrogen Tank Rental	$0 /mo/tank	HYD2
Liq Carrier Gas Tank Rental	$0 /mo/tank	CAR2
Gas Storage Equipment Rent	$0 /year	GTANK2
Machine Cost	$1,000,309 /sta	MCH2B
Installed Equipment Cost	$1,350,417 /sta	IEQUIP2
Auxiliary Equipment Cost	$150,046 /sta	AEQUIP2
Equipment Annuity	$3,632,131 /yr	EINT2

Tooling Annuity	$76,489 /yr	TINT2
Building Annuity	$43,978 /yr	BINT2
Working Annuity	$3,205,157 /yr	WINT2

| MICROWAVE CVD TCM: | COST SUMMARY |
| IBIS ASSOCIATES, INC. | Copyright (c) 1996 v4.0 |

	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$859.17	$859,165	12.3%	
Direct Labor Cost	$147.65	$147,653	2.1%	
Utility Cost	$951.88	$951,885	13.7%	
FIXED COST ELEMENTS				
Equipment Cost	$2,849.13	$2,849,127	40.9%	$15,004,630
Tooling Cost	$60.00	$60,000	0.9%	$300,000
Building Cost	$18.99	$18,988	0.3%	$400,000
Maintenance Cost	$1,170.03	$1,170,032	16.8%	
Overhead Labor Cost	$23.74	$23,735	0.3%	
Cost of Capital	$877.17	$877,170	12.6%	
TOTAL FABRICATION COST	$6,957.76	$6,957,755	100.0%	$15,704,630

SUMMARY INFORMATION

Part Name	20 in. substrate	
Total Direct Laborers	6.00	/shift
Total Floor Space	5,350	sqft
Total Capital Investment	$15.7	MM
Area Cost	$3.39	/sqcm
Cost Per Carat	$3.87	/ct
Number of Carats Per Wafer	1799.34	carats/wafer
Machine Throughput	189,471	ct/year/mch

Appendix C: The Combustion Flame TCM

COMBUSTION FLAME CVD DIAMOND TECHNICAL COST MODEL - LONG TERM
IBIS ASSOCIATES, INC.   Copyright (c) 1996 v4.0

Revision Date: 4/96

PRODUCT SPECIFICATIONS

Torch Type	Single Nozzle	
Part Name	4 in. substrate	NAME
Wafer Diameter	8.90 cm	DIAM
Finished Wafer Thickness	500 um	THIK
Thermal Conductivity	1,000 W/mK	THERMCON
Annual Production Volume	1.0 (000/yr)	NUM
Length of Production Run	5 yrs	PLIFE

PROCESS RELATED FACTORS - DEPOSITION

Process In Use?	1 [1=Y 0=N]	USE2
Dedicated Investment	0 [1=Y 0=N]	DED2
Process Yield	90.0%	YLD2
Average Equipment Downtime	15.0%	DOWN2
Direct Laborers	0.10 /sta	NLAB2
Machine Power	2 kW	POW2
Machine Load/Unload Time	120 min/batch	PTIME2
Available Deposition Time	8,640 hrs/yr	DAYHR2
Heat Removal via Substrate	50.0% of total	HTRMV2
Coolant Temp. Rise	50 C	TEMP2
Heat Capacity of Coolant	1.0 cal/g/C	CP2
Building Space Requirement	200 sqft/sta	FLR2
Acetylene:Oxygen Ratio (R)	1.02 [1.02<x<1.1]	GRATIO2
Oxygen	26 [menu #]	GASA2
Acetylene	20 [menu #]	GASB2
Oxygen Recycle Rate	0.0%	RECYC2A
Carrier Gas Recycle Rate	0.0%	RECYC2B
Gas Recycle Equipment Cost	NA total	MCH2A
Substrate:Duct Area Ratio	3.00 [1<x<=4]	SUBDUC2
Substrate Distance:Duct Diam	1.00 [0<x<=10]	L:D2

EXOGENOUS COST FACTORS

Direct Wages	$13.33 /hr	WAGE
Indirect Salary	$50,000 /yr	SALARY
Indirect:Direct Labor Ratio	0.50	ILAB
Benefits on Wage and Salary	35.0%	BENI
Working Days per Year	360	DAYS
Working Hours per Day	24 hr	HRS

Capital Recovery Rate	10%	CRR
Capital Recovery Period	5 yrs	ELIFE
Building Recovery Life	20 yrs	BLIFE
Working Capital Period	3 months	WCP
Price of Electricity	$0.050 /kWh	ELEC
Price of Natural Gas	$6.50 /MBTU	GAS
Price of Building Space	$100 /sqft	PBLD
Price of Cooling Water	$0.03 /100 gal	WATER
Auxiliary Equipment Cost	15.0%	AUX
Equipment Installation Cost	35.0%	INST
Maintenance Cost	8.0%	MNT

	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$783.43	$783,425	64.7%	
Direct Labor Cost	$74.52	$74,516	6.2%	
Utility Cost	$5.72	$5,719	0.5%	
FIXED COST ELEMENTS				
Equipment Cost	$179.68	$179,677	14.8%	$937,500
Tooling Cost	$0.00	$0	0.0%	$0
Building Cost	$4.79	$4,791	0.4%	$100,000
Maintenance Cost	$79.54	$79,537	6.6%	
Overhead Labor Cost	$11.98	$11,978	1.0%	
Cost of Capital	$71.65	$71,649	5.9%	
TOTAL FABRICATION COST	$1,211.29	$1,211,293	100.0%	$1,037,500

INTERMEDIATE CALCULATIONS

Process In Use	1	[1=Y 0=N]	PRO2
Cumulative Yield	90.0%		CYLD2
Effective Production Volume	1,111	/yr	ENUM2
Machine Power	2	kW	DAPOW2
Duct Area (A inf.)	20.74	sqcm	DAREA2
Duct Diameter	5.14	cm	DDIAM2
Quality Multiplier	1.07	[0.4<x<5]	QMULT2
Strain Rate (a)	412	1/sec	STRN2A
Atomic Hydrogen Concentr.	2.82E-09	mol/cc	HCONC2
H/CH3 Ratio at Substrate	10.89		HRATIO2
Methyl (CH3) Concentr.	2.59E-10	mol/cc	MCONC2
Volume Expansion Factor	7.40		VOLEF2A
Gas Velocity	2,103	cm/s	SPEED2A
Total Gas Flow Rate	354	slm	TFLOW2A
Acetylene Flow Rate	179	slm	CFLOW2A
Oxygen Gas Flow Rate	175	slm	XFLOW2A
Mass of Diamond Deposited	10.92	g	MASS2
Linear Deposition Rate	16.9	um/hr	LINDEP2
Mass Deposition Rate	0.4	g/hr	MASDEP2
Deposition Time	29.67	hrs	CTIMEB2
Machine Setup Time	2.00	hrs	CTIMEA2
Single Machine Productivity	231	wafers/year	SMPR2

Runtime for One Station	479%	RTIME2
Number of Parallel Stations	4.79	NSTAT2
Total Oxygen Gas Volume	312 SCM/pc	XGAS2
Total Carbon Gas Volume	318 SCM/pc	CARGAS2
Oxygen Gas Cost	$65 /pc	COSTA2
Acetylene Gas Cost	$636 /pc	COSTB2
Carbon Capture Factor	0.0035%	CCF2
Combustion Enthalpy Change	-447 kJ/mol	ENTH2
Mass Flow of C2H2 and O2	0.24 mol/sec	MFLOW2
Combustion Eff. Power	108 kW	CPOW2
Cooling Water Flow Rate	4.1 gal/min	WATER2
Cooling Water Requirement	7,267 gal/pc	COOL2
Energy Requirement	59 kWh/pc	ENERGY2
Building Space/Station	200 sqft	SPACE2
Recycle Equipment Cost	$0 /sta	REC2
Liquid Oxygen Tank Rental	$350 /mo/tank	XRENT2
Gas Storage Equipment Rent	$4,200 /year	GTANK2
Machine Cost	$125,000 /sta	MCH2B
Installed Equipment Cost	$168,750 /sta	IEQUIP2
Auxiliary Equipment Cost	$18,750 /sta	AEQUIP2
Equipment Annuity	$229,057 /yr	EINT2
Tooling Annuity	$0 /yr	TINT2
Building Annuity	$11,097 /yr	BINT2
Working Annuity	$971,139 /yr	WINT2

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COMBUSTION CVD TCM:    COST SUMMARY
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	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$783.43	$783,425	64.7%	
Direct Labor Cost	$74.52	$74,516	6.2%	
Utility Cost	$5.72	$5,719	0.5%	
FIXED COST ELEMENTS				
Equipment Cost	$179.68	$179,677	14.8%	$937,500
Tooling Cost	$0.00	$0	0.0%	$0
Building Cost	$4.79	$4,791	0.4%	$100,000
Maintenance Cost	$79.54	$79,537	6.6%	
Overhead Labor Cost	$11.98	$11,978	1.0%	
Cost of Capital	$71.65	$71,649	5.9%	
TOTAL FABRICATION COST	$1,211.29	$1,211,293	100.0%	$1,037,500

SUMMARY INFORMATION

Part Name	4 in. substrate	
Total Direct Laborers	5.50	/shift
Total Floor Space	2,350	sqft
Total Capital Investment	$1.0	MM
Area Cost	$19.47	/sqcm
Cost Per Carat	$22.19	/ct
Number of Carats Per Wafer	54.59	carats/wafer
Machine Throughput	11,349	ct/year/mch

Appendix D: Upper Bound on Growth Rate Analysis

An Upper Bound for the Growth Rate of CVD Diamond

D. G. Goodwin
March 19, 1996

In order to assess the lowest long-term cost for CVD diamond, it is useful to have an estimate of the highest possible theoretical growth rate. This report summarizes an analysis which allows this upper-bound growth rate to be determined.

Diamond Growth Chemistry

In order to understand the factors which limit diamond growth rates and quality, it is first necessary to know how film properties are related to the gas-phase environment at the substrate.

It is now generally accepted that the methyl radical CH_3 is the principal gas-phase precursor to diamond in most CVD environments (Harris and Weiner, 1991; Harris and Martin, 1990; D'Evelyn et al., 1992). Some other possible precursors have been postulated as well, including C_2H_2, C, and C_2. However, the conditions under which these species could play a role are limited, and do not reflect "standard" diamond CVD conditions.

While there is still uncertainty regarding the details of the mechanism by which diamond grows from the vapor phase, the qualitative features are now well-understood. The most significant feature of essentially all diamond CVD environments is that the growing diamond surface is exposed to a large flux of atomic hydrogen, which plays several roles in the diamond growth process.

The first consequence of the presence of H in the gas-phase is that the diamond surface is primarily terminated with C-H bonds, which maintains the sp^3 diamond lattice structure. However, due to the constant bombardment by H, some of these surface-bonded H are abstracted:

$$C_dH + H \rightarrow C_d^* + H_2. \tag{1}$$

Here C_dH represents a hydrogenated diamond surface site, and C_d^* an empty, or dangling-bond surface site. Since the H-H bond strength is greater than the C-H bond strength, this process is exothermic. It also has a relatively

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low activation energy ($\approx$ 7 kcal/mol) and thus proceeds readily. A second process can occur in which atomic hydrogen recombines on an open radical site:

$$C_d^* + H \rightarrow C_dH. \tag{2}$$

Under CVD conditions, both of these processes occur rapidly, resulting in a dynamic balance which leads to a steady-state fraction f^* of open radical sites. Since the rates for both of these processes are proportional to the H concentration, the value of f^* is independent of [H]. It may be shown to be equal to

$$f^* = \frac{\gamma_a}{\gamma_a + \gamma_r}, \tag{3}$$

where γ_a is the probability that an incident H atom will abstract a surface H, and γ_r is the probability that an H atom incident on a radical site will recombine with it. The best estimates for γ_a and γ_r indicate that the open fraction f^* is a few percent up to perhaps 20% at typical diamond CVD temperatures (Goodwin, 1993a).

Diamond growth occurs when gas-phase carbon-bearing reactive species (e.g. CH_3) react with a surface dangling-bond site to form a surface species. This surface species is incorporated into the diamond lattice through a sequence of H-abstraction reactions with gas-phase H which remove the remaining hydrogen atoms, allowing bonds to form with neighboring carbons. This description is highly simplified; for detailed analyses see, for example, Garrison et al. (1992); Harris (1990); Harris and Goodwin (1993); Huang and Frenklach (1992).

In addition to its roles in providing open surface sites and abstracting H during the carbon incorporation process, H plays another role which is the decisive one enabling CVD diamond growth. Exposing a diamond surface to a flux of reactive carbon species (or hydrocarbons) is not sufficient by itself to continue diamond growth; instead, an amorphous or graphitic layer would quickly result. Some means is required to suppress the thermodynamically-stable graphitic phase to allow the metastable diamond phase to grow.

Atomic hydrogen is known to be able to etch graphite films and amorphous carbon films (Rye, 1977), but no measurable etch rate for diamond has ever been reported. As discussed by Butler and Woodin (1993) and others, H is able to attack graphite or amorphous carbon through insertion into unsaturated C=C bonds, followed by a chemical process known as β-scission. The diamond structure, on the other hand, is stable with respect to β-scission

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since every surface atom is bonded to 3 others by single C-C bonds.

Simplified models of the competition between diamond growth, deposition of non-diamond carbon, and etching of non-diamond carbon by H indicate that the ratio of the H flux striking the surface to the diamond growth rate should be an important variable determining diamond quality, along with substrate temperature (Butler and Woodin, 1993; Goodwin, 1993b).

It is convenient to recast the film linear growth rate in terms of the number of carbon atoms added to the diamond film per unit area per unit time. The non-dimensional parameter determining quality is then the ratio of the incident H flux to the carbon incorporation rate. We will call this ratio N.

The atomic hydrogen flux to the surface (or equivalently, the concentration at the surface) is difficult to measure, since H recombines rapidly on the surface leading to sharp concentration gradients in the gas-phase above the substrate. Most studies which report diamond growth results do not attempt to estimate the H flux incident on the surface.

In order to obtain estimates for the N parameter, atomic hydrogen fluxes have been estimated for a variety of different diamond growth techniques reported in the literature, summarized in Table I. For the hot-filament case, the H concentration at the substrate was measured (Hsu, 1991). In all others, it was estimated based on the stated growth conditions. In some cases, these estimates are the results of detailed numerical simulations, while in others (e.g. microwave) a simple power balance on the plasma was used to estimate the H production rate, which balances the loss rate on the substrate.

The H flux estimates are compared in Table I to the experimental diamond growth rates reported in these studies, and the N parameter is calculated. The results in Table I show that widely-varying diamond growth methods all require a value of $N \sim 10^4$ in order to grow diamond.

In general, we would expect that the diamond quality would increase for higher N, and degrade for lower N. In most of these experiments, diamond with a sharp 1332 cm^{-1} Raman line was grown, but its quality (as measured, for example, by thermal conductivity) was not extensively analyzed. It is reasonable to take the value of $N \approx 10^4$ as the *minimum* N value necessary for diamond growth.

This analysis is supported also by the experiments of Olson et al. (1994). In these experiments, diamond was grown by exposing a substrate alternately to a carbon flux and then to an atomic hydrogen flux. While these conditions of course differ from standard CVD conditions, they provide a degree of

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Experiment	Pressure	H flux (cm^{-2})	G $(\mu\text{m/hr})$	$\log_{10} N$
Stagnation-point flame (Murayama and Uchida, 1992) (Meeks et al., 1993)	1 atm	9×10^{20}	40	3.67
Flat Flame (Glumac and Goodwin, 1992)	52 Torr	6×10^{19}	1	4.1
Hot Filament (Hsu, 1991)	20 Torr	4×10^{19}	0.5	4.2
Astex Microwave	~ 120 Torr	2×10^{21}	13.5	4.6
RF Torch (Girshick et al., 1993)	1 atm	8×10^{20}	17	4.0
DC Arcjet (Stalder and Sharpless, 1990)	220 Torr	7×10^{21}	60	4.4

control not possible with standard methods. Olson et al. report the type of carbon deposit (either disordered carbon or diamond particles) as a function of two parameters: the number of monolayers of carbon exposure per cycle, and the number of monolayers of atomic hydrogen exposure per cycle.

The transition from disordered carbon to diamond is found to occur at a hydrogen/carbon exposure ratio of roughly 3×10^3. If it is assumed (as they do) that only some fraction of the incident carbon flux is incorporated, this is consistent with an N parameter of order 10^4.

Atomic Hydrogen Transport

Since the achievable diamond growth rate (at acceptable quality) is directly proportional to the H flux delivered to the substrate, the conditions which maximize growth rate will be those which deliver the highest possible flux of atomic hydrogen to the substrate.

Goodwin (1993b) has recently carried out an in-depth analysis of the question of H transport under CVD diamond conditions. Results of this analysis will be summarized here, and used to estimate an upper-bound growth rate.

Depending on reactor type and operating conditions, H may be supplied to the substrate either by diffusion or convection. Typically, hot-filament and microwave systems operate in a diffusive mode, while combustion, arcjet, and RF torch methods utilize convective transport. Generally, the highest fluxes

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can be achieved in convective reactors, and these will be the focus of this analysis.

As shown by Goodwin (1993b), H recombines on the diamond surface fast enough that H-transport to the surface is usually diffusion-limited under most diamond CVD conditions. [The probability that an H atom will recombine to H_2 upon striking a diamond surface is roughly 0.1 (Harris and Weiner, 1993).]

For a convective process, a thin concentration boundary layer develops over the substrate, in which the H concentration drops off sharply from the value in the gas-phase outside the boundary layer to a lower value at the substrate. The concentration at the substrate is maintained by the balance between supply of H and surface recombination of H.

The flux of H to the substrate may be written as

$$j_H = \frac{n_0 D_H}{\delta_H} \left(X_{H,\infty} - X_{H,0} \right) \tag{4}$$

where n_0 is the number density in the gas (molecules/cm^3), D_H is the diffusion coefficient of atomic hydrogen (cm^2/s), δ_H is the boundary layer thickness, and X_H is the atomic hydrogen mole fraction. The subscript ∞ denotes a location outside the boundary layer, and the subscript zero denotes the value at the substrate.

Equation 4 neglects any recombination of H within the boundary layer. At sufficiently low pressure this is justified. We will address the question of the pressure at which recombination sets in below.

The H mole fraction at the surface is given by

$$\frac{X_{H,0}}{X_{H,\infty}} = \frac{1}{1 + \gamma_H \delta_H / \lambda_H}, \tag{5}$$

where γ_H is the surface recombination probability and λ_H is defined by

$$\lambda_H = \frac{4 D_H}{\bar{c}_H} \tag{6}$$

and is approximately equal to the mean free path of an H atom. In this expression, $\bar{c}_H$ is the mean thermal speed of an H atom.

There are two primary ways to maximize the flux j_H. The product $n_0 D_H$ is independent of pressure and only weakly temperature dependent, so this

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term in equation 4 cannot be substantially altered. This leaves two possibilities: either minimize δ_H, or maximize $X_{H,\infty}$. (Recall that $X_{H,0}$ is determined by equation 5, and thus is not a free parameter.)

Maximizing $X_{H,\infty}$ means increasing the H_2 dissociation fraction to the largest possible value (ideally producing full dissociation). This can be done with a high-power microwave system, or using a thermal plasma with a temperature of order 5000 K.

Assuming the hydrogen is maximally dissociated, the only possibility left is to decrease the boundary layer thickness δ_H. For an axisymmetric stagnation point, the boundary layer thickness is given by

$$\delta_H = 1.32 \left(\frac{\nu}{a}\right)^{1/2} \left(\frac{D_H}{\nu}\right)^{0.4}. \tag{7}$$

Here ν is the kinematic viscosity of the gas.

The quantity a is known as the stagnation-point strain rate, and is proportional to the incident gas speed U_∞ divided by the substrate diameter d_s:

$$a = C \frac{U_\infty}{d_s}. \tag{8}$$

The constant C depends on the substrate geometry and flow characteristics, but for a disk is in the range from 0.3 to 1.3.

Putting in numerical values for gas properties appropriate for a dilute hydrocarbon/hydrogen mixture, equation 7 becomes

$$\delta_H \approx \frac{160}{\sqrt{ap}} \text{ cm}, \tag{9}$$

with a in cm^{-1} and p in Torr. This expression indicates that to minimize the boundary layer thickness one should maximize a, or p, or both.

It may be shown that there is a maximum achievable a parameter (Goodwin, 1993b). The maximum value is approximately given by

$$a_{max} \approx \frac{1}{d_s} \left(\frac{RT_\infty}{m}\right)^{1/2}, \tag{10}$$

where m is the gas molecular weight. For a 10 cm diameter substrate, an upper-bound gas temperature of 10,000 K, and a lower-bound molecular weight of 1, this reduces to

$$a_{max} \approx 10^5 \text{ s}^{-1}. \tag{11}$$

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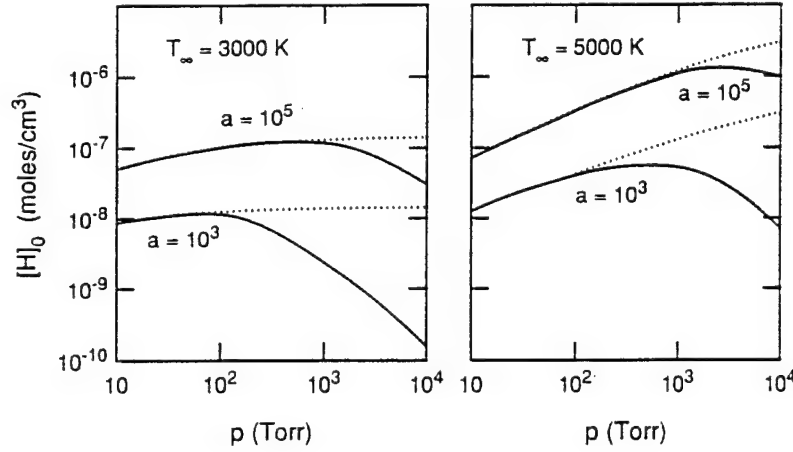
Figure 1: H concentration at the substrate vs pressure at fixed a and T_∞, assuming chemical equilibrium exists outside the boundary layer. The dashed curves show the results if boundary-layer chemistry is neglected.

This expression for a_{max} determines the minimum possible boundary layer thickness for a given pressure.

The above analysis neglected the possibility of homogeneous recombination of H to H_2 within the boundary layer. This is reasonable at low pressure, but beyond some pressure H will be lost due to homogeneous recombination and the H flux will be reduced compared to that estimated above.

Goodwin (1993b) has carried out detailed numerical simulations to investigate this effect. The simulation results are reproduced in Figure 1. For $T_\infty = 5000$ K and $a = 10^5$ s^{-1}, the simulations show that the H concentration at the substrate increases with pressure until a pressure of roughly 2000 Torr, at which point it begins to decline due to homogeneous recombination.

The maximum achievable concentration at the substrate is found to be approximately 6×10^{17} cm^{-3}. Converting this to a flux, this corresponds to

$$j_{H,max} \approx 7 \times 10^{22} \text{ cm}^{-2}\text{s}^{-1}. \tag{12}$$

We may now use this result to estimate the maximum achievable growth rate. If we take $N = 10^4$, then the maximum possible incorporated carbon flux is

$$j_{C,max} \approx 7 \times 10^{18} \text{ cm}^{-2}\text{s}^{-1}. \tag{13}$$

Converting this value to a linear growth rate results in

$$G_{max} = 1.5 \text{ mm/hr}. \tag{14}$$

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We therefore conclude that a rate of 1.5 mm/hr is an absolute upper bound to the CVD diamond growth rate, based simply on the maximum flux of H which may be delivered by means of convection to a substrate.

The methyl concentration which would be required to achieve this growth rate may be estimated by the approximate relation (Goodwin, 1993a)

$$G = 1.8 \times 10^{11} \frac{[CH_3][H]}{5.0 \times 10^{-9} + [H]} \tag{15}$$

where the growth rate is in microns per hour and the concentrations are in moles/cm^3. Using G_{max} and the H concentration estimated above results in

$$[CH_3] \approx 8.3 \times 10^{-9} \text{ moles/cm}^3, \tag{16}$$

which corresponds to a CH$_3$ mole fraction at the substrate of 4×10^{-4}.

Of course, the conditions required to achieve this maximum growth rate are extreme, and would produce very large substrate heat fluxes. Such heat fluxes would pose difficult temperature control problems. In addition, the stress produced in the film under these high-rate conditions might lead to low yields. It is likely that factors such as these would limit the actual achievable growth rate to a value significantly below this theoretical maximum.

References

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Appendix E: The Lowest Foreseeable Cost TCM

Revision Date: 4/96

PRODUCT SPECIFICATIONS

Part Name Lowest foreseeable cost		NAME
Wafer Diameter	110.00 cm	DIAM
Finished Wafer Thickness	500 um	THIK
Thermal Conductivity	1,000 W/mK	THERMCON
Annual Production Volume	1.0 (000/yr)	NUM
Length of Production Run	5 yrs	PLIFE

PROCESS RELATED FACTORS - DEPOSITION

Process In Use?	1 [1=Y 0=N]	USE2
Dedicated Investment	0 [1=Y 0=N]	DED2
Process Yield	90%	YLD2
Average Equipment Downtime	15%	DOWN2
Direct Laborers	0.40 /sta	NLAB2
Machine Power	925 kW	POW2
Power to Gas Efficiency	100%	P2GEFF
Machine Load/Unload Time	15 min/batch	PTIME2
Available Deposition Time	8,640 hrs/yr	DAYHR2
Coolant Temp. Rise	50 C	TEMP2
Heat Capacity of Coolant	1.0 cal/g/C	CP2
Building Space Requirement	1,500 sqft/sta	FLR2
Reactor Pressure	50 torr	RPRESS
Substrate Temperature	1,173 K	STEMP
Gas Temperature (>1000K)	5,000 K	GTEMP
Hydrogen Gas Flow Rate	1,973.6 slm	HFLOW
Carbon Gas Flow Rate	19.7 slm	CFLOW
Argon Gas Flow Rate	0.0 slm	ARFLOW
Other Gas Flow Rate	0.0 slm	OGFLOW

Total Gas Flow Rate	1,993.3 slm	

	Menu #	vol%	
Hydrogen	3	99.0%	GASA VOLA
Carbon Containing Gas	16	1.0%	GASB VOLB

Carrier Gas	0	0.0%	GASC VOLC
Other Gas	0	0.0%	GASD VOLD
		100.0%	

Hydrogen Recycle Rate	0%	RECYC
Carrier Gas Recycle Rate	0%	RECYC2
Gas Recycle Equipment Cost	$250,000 total	MCH2A
Recombine Coef. (gammaH)	0.10	RECOMBX
Substrate:Duct Area Ratio	3.00	SUBDUCT
Substrate Shape Factor (c)	1.00	SHAPFAC
Diamond Density	3.51 g/cc	DENS
Ideal Gas Constant (R)	62,358 cc torr/K mol	IDEALG1
Ideal Gas Constant 2 (R)	8.31 J / mol K	IDEALG2

NASA Enthalpy Constants	H2	H	Ar
a1	2.99E+00	2.50E+00	2.50E+00
a2	7.00E-04	0.00E+00	0.00E+00
a3	-5.63E-08	0.00E+00	0.00E+00
a4	-9.23E-12	0.00E+00	0.00E+00
a5	1.58E-15	0.00E+00	0.00E+00
a6	-8.35E+02	2.55E+04	-7.45E+02
a7	-1.36	-0.46	4.37
MW	2.02	1.01	39.95

EXOGENOUS COST FACTORS

Direct Wages	$13.33 /hr	WAGE
Indirect Salary	$50,000 /yr	SALARY
Indirect:Direct Labor Ratio	0.50	ILAB
Benefits on Wage and Salary	35%	BENI
Working Days per Year	360	DAYS
Working Hours per Day	24 hr	HRS
Capital Recovery Rate	10%	CRR
Capital Recovery Period	5 yrs	ELIFE
Building Recovery Life	20 yrs	BLIFE
Working Capital Period	3 months	WCP
Price of Electricity	$0.050 /kWh	ELEC
Price of Natural Gas	$6.50 /MBTU	GAS
Price of Building Space	$100 /sqft	PBLD
Price of Cooling Water	$0.03 /100 gal	WATER
Auxiliary Equipment Cost	15%	AUX
Equipment Installation Cost	35%	INST
Maintenance Cost	8%	MNT

	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$1,052.54	$1,052,542	29.7%	
Direct Labor Cost	$165.63	$165,633	4.7%	
Utility Cost	$915.81	$915,814	25.9%	
FIXED COST ELEMENTS				
Equipment Cost	$752.35	$752,351	21.2%	$4,238,500
Tooling Cost	$0.00	$0	0.0%	$0
Building Cost	$19.97	$19,969	0.6%	$450,000
Maintenance Cost	$332.89	$332,891	9.4%	
Overhead Labor Cost	$26.63	$26,626	0.8%	
Cost of Capital	$274.72	$274,717	7.8%	
TOTAL FABRICATION COST	$3,540.54	$3,540,543	100.0%	$4,688,500

INTERMEDIATE CALCULATIONS

Process In Use	1.00	[1=Y 0=N]	PRO2
Cumulative Yield	90.0%		CYLD2
Effective Production Volume	1,111	/yr	ENUM2

ENERGY BALANCE CALCULATIONS

	H2	H	Ar	
Enthalpy Per Unit Mass	82,789	313,233	2,446	J/g
Molar Enthalpy	166,887	315,707	97,731	J/mol
Molar Entropy	222.67	173.21	213.34	J/K mol
Molar Heat Capacity (Cp)	40.89	20.79	20.79	J/K mol

Heat of Reaction (H2==>2H)	464,528	J/mol
Entropy of Rxn (H2==>2H)	124	J/K mol
Free Energy of Rxn (H2==>2H)	(154,204)	J/mol
Equilibr Const Kp (H2==>2H)	4.08E+01	

Mole Fraction H	99.84%
Mole Fraction Argon	0.00%
Mole Fraction H2	0.16%

Total Molar Enthalpy	315,468 J/mole	
Mean Molecular Weight	1.01 g/mole	
Mean Specific Enthalpy	312,494 J/g	
Mean Molar Heat Capacity	20.82 J/K mol	
Deposition Arc Power	925 kW	DAPOW2
Duct Area (A inf.)	3,167.77 sqcm	DCTAREA
Duct Diameter	63.51	DCTDIAM
Mass Flux	2.96 g/s	
Gas Velocity (U inf.)	5,772 cm/s	
Specific Heat Ratio (gamma)	1.66	
Speed of Sound	828,019 cm/s	
Mach Number	0.01	

Note: Adjust Input Temperature (cell B47) or gas flow rates such that Temp. Solver = 0

Input Temperature	5,000 K
Temperature Solver	-2.91E-11

BOUNDARY LAYER CALCULATIONS

Strain Rate (a)	91 1/s
Gas Pressure at Substrate	50.00 torr
Hydrogen Boundary Layer	2.37 cm
Thermal Boundary Layer	2.08 cm
H Mean Free Path (lambda)	2.80E-03 cm
Knudsen Number	1.18E-03
H Mole Fraction at Substrate	1.16%
H Concentration at Substrate	7.96E-09 mol/cc
H/CH3 Ratio	10.89
CH3 Concentration at Substr.	7.31E-10 mol/cc

DEPOSITION RATE CALCULATIONS

Mass of Diamond Deposited	1667.83 g	MASS2
Linear Deposition Rate	28.8 um/hr	LINDEP2
Mass Deposition Rate	96.1 g/hr	MASDEP2
Deposition Time	17.35 hrs	CTIMEB2
Machine Setup Time	0.25 hrs	CTIMEA2
Single Machine Productivity	417 wafers/year	SMPR2
Runtime for One Station	266%	RTIME2
Number of Parallel Stations	2.66	NSTAT2

Total Hydrogen Gas Volume	2054.29 SCM	HGAS2
Total Argon Gas Volume	0.00 SCM	ARGAS2
Total Carbon Gas Volume	20.54 SCM	CARGAS2
Total Gas Volume	2,075 SCM	TVOL2
Total Gas Flow Rate	1,993,293 sccm	FLOWR2
Carbon Capture Factor	16.54%	CCF2

	Consumption (SCM/pc)	Cost ($/pc)		
Hydrogen Consumption	2054.29	$616.29	GASA2	COSTA2
Carbon Gas Consumption	20.54	$282.67	GASB2	COSTB2
Carrier Gas Consumption	0.00	$0.00	GASC2	COSTC2
Other Gas Consumption	0.00	$0.00	GASD2	COSTD2
Energy Requirement	16,047 kWh/pc		ENERGY2	
Cooling Water Flow Rate	70.0 gal/min		WATER2	
Cooling Water Requirement	72,887 gal/pc		COOL2	
Building Space/Station	1,500 sqft		SPACE2	
Recycle Equipment Cost	$0 /sta		REC2	
Liquid Hydrogen Tank Rental	$4,475 /mo/tank		HYD2	
Liq Carrier Gas Tank Rental	$0 /mo/tank		CAR2	
Gas Storage Equipment Rent	$53,700 /year		GTANK2	
Machine Cost	$941,889 /sta		MCH2B	
Installed Equipment Cost	$1,271,550 /sta		IEQUIP2	
Auxiliary Equipment Cost	$141,283 /sta		AEQUIP2	
Equipment Annuity	$959,114 /yr		EINT2	
Tooling Annuity	$0 /yr		TINT2	
Building Annuity	$46,250 /yr		BINT2	
Working Annuity	$2,535,179 /yr		WINT2	

	per piece	per year	percent	investment
VARIABLE COST ELEMENTS				
Material Cost	$1,052.54	$1,052,542	29.7%	
Direct Labor Cost	$165.63	$165,633	4.7%	
Utility Cost	$915.81	$915,814	25.9%	
FIXED COST ELEMENTS				
Equipment Cost	$752.35	$752,351	21.2%	$4,238,500
Tooling Cost	$0.00	$0	0.0%	$0
Building Cost	$19.97	$19,969	0.6%	$450,000
Maintenance Cost	$332.89	$332,891	9.4%	
Overhead Labor Cost	$26.63	$26,626	0.8%	
Cost of Capital	$274.72	$274,717	7.8%	
TOTAL FABRICATION COST	$3,540.54	$3,540,543	100.0%	$4,688,500

SUMMARY INFORMATION

Part Name	Lowest foreseeable cost	
Total Direct Laborers	6.20	/shift
Total Floor Space	5,850	sqft
Total Capital Investment	$4.7	MM
Area Cost	$0.37	/sqcm
Cost Per Carat	$0.42	/ct
Number of Carats Per Wafer	8339.16	carats/wafer
Number of Carats Per Year	3,129,687	ct/year/mch

Appendix F: CVD Diamond Survey

CVD Diamond Questionnaire
What is state-of-the-art and how much will happen in five years?

1. For all of the technologies, make suggested changes for the following assumptions in the spaces provided:

Assumption		Microwave (Now)	Microwave (+5 Yrs)	DC Arcjet (Now)	DC Arcjet (+5 Yrs)	Combustion (Now)	Combustion (+5 Yrs)
Equipment Price ($000/station)	current	945	2,026	675	976	61	96
	suggested						
Deposition Yield	current	75%	85%	75%	90%	88%	90%
	suggested						
Overall Yield (includes finishing)	current	68%	78%	72%	87%	74%	87%
	suggested						
Deposition Rate (microns per hour)	current	8	22	17	20	35	40
	suggested						
Equipment Power (kW per station)	current	75	500	50	125	N/A	N/A
	suggested						

2. Please comment on the other inputs in the table and the graphs that are provided.

3. What is the "best case scenario" for CVD diamond manufacturing (assume thermal conductivity of about 1,000 W/mK) that would lead to its lowest foreseeable cost, in your opinion? Please note which deposition technology is being considered.

	Units	Low Estimate	Probable Value	High Estimate
Equipment Price				
Deposition Yield				
Overall Yield				
Deposition Rate				
Equipment Power				

IBIS Associates, Inc.

	Microwave 1996	Microwave 2001	DC Arcjet 1996	DC Arcjet 2001	Flame 1996	Flame 2001
SELECTED INPUTS						
Wafer Thickness (u)	500	500	500	500	500	500
Thermal Conductivity (W/mK)	1,000	1,000	1,000	1,000	1,000	1,000
Machine Power (kW)	75	500	50	125	NA	NA
Laborers Per Station	0.1	0.1	0.1	0.1	0.1	0
Floorspace Per Station (sqft)	400	400	1,500	1,500	1,500	1,500
Total Gas Flow Rate (slm)	4	68	111	369	230	2,070
Gas Mix % (H2 / CH4 / O2 / C2H2)	89 / 1 / 10 / -	89 / 1 / 10 / -	99 / 1 / - / -	99 / 1 / - / -	22 / - / 38 / 40	22 / - / 38 / 40
Deposition Yield (%)	75%	85%	75%	90%	88%	90%
COMPUTED VALUES						
Wafer Diameter (cm)	22.1	57.1	17.8	30.5	5.1	15.2
Mass Deposition Rate (g/hr)	1.1	20.0	1.5	5.0	0.2	2.6
Linear Deposition Rate (u/hr)	8	22	17	20	35	40
Deposition Cycle Time (hrs)	61	23	34	29	16	15
Machine Cost ($/sta)	$944,982	$2,025,979	$675,332	$976,088	$60,668	$96,012
Good Wafer Yield (%)	68%	78%	72%	86%	74%	86%

IBIS
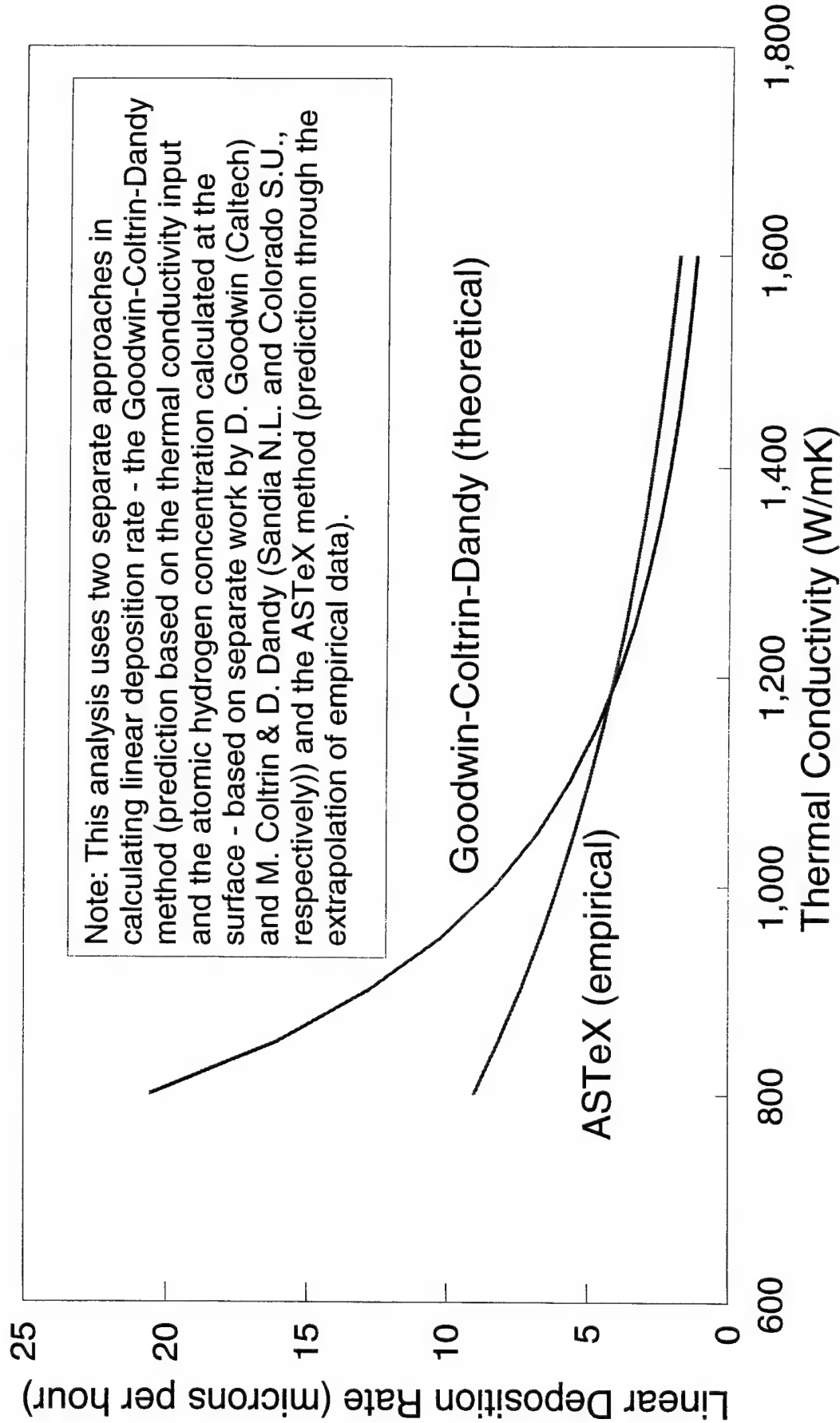
Note: These assumptions serve only as a starting point for discussion and do not represent the opinion of IBIS Associates, Inc.

Preliminary Analysis

Cost Vs. Deposition Diameter
Combustion Flame Deposition - Today

Total Gas Flow Rate (SCM per minute)

Deposition Diameter (cm)

Deposition Cost Per Carat

Preliminary Analysis

IBIS Associates, Inc.
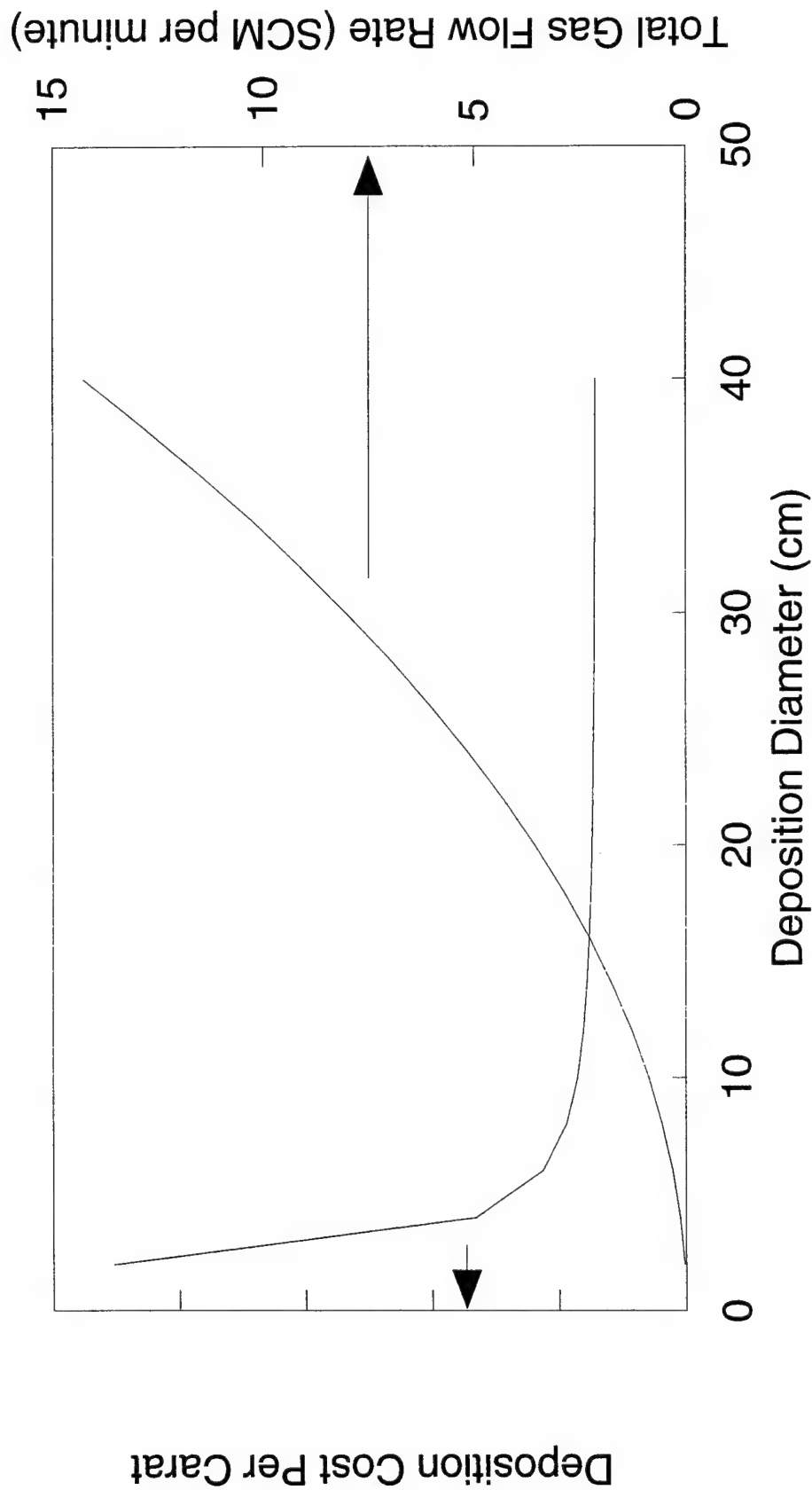
Deposition Rate vs. Thermal Conductivity

Note: This analysis uses two separate approaches in calculating linear deposition rate - the Goodwin-Coltrin-Dandy method (prediction based on the thermal conductivity input and the atomic hydrogen concentration calculated at the surface - based on separate work by D. Goodwin (Caltech) and M. Coltrin & D. Dandy (Sandia N.L. and Colorado S.U., respectively)) and the ASTeX method (prediction through the extrapolation of empirical data).

Goodwin-Coltrin-Dandy (theoretical)

ASTeX (empirical)

Linear Deposition Rate (microns per hour)

25 — 20 — 15 — 10 — 5 — 0

Thermal Conductivity (W/mK)

600   800   1,000   1,200   1,400   1,600   1,800

Cost & Area vs. Power

DC Arcjet Deposition - Today

IBIS Associates, Inc.

Preliminary Analysis
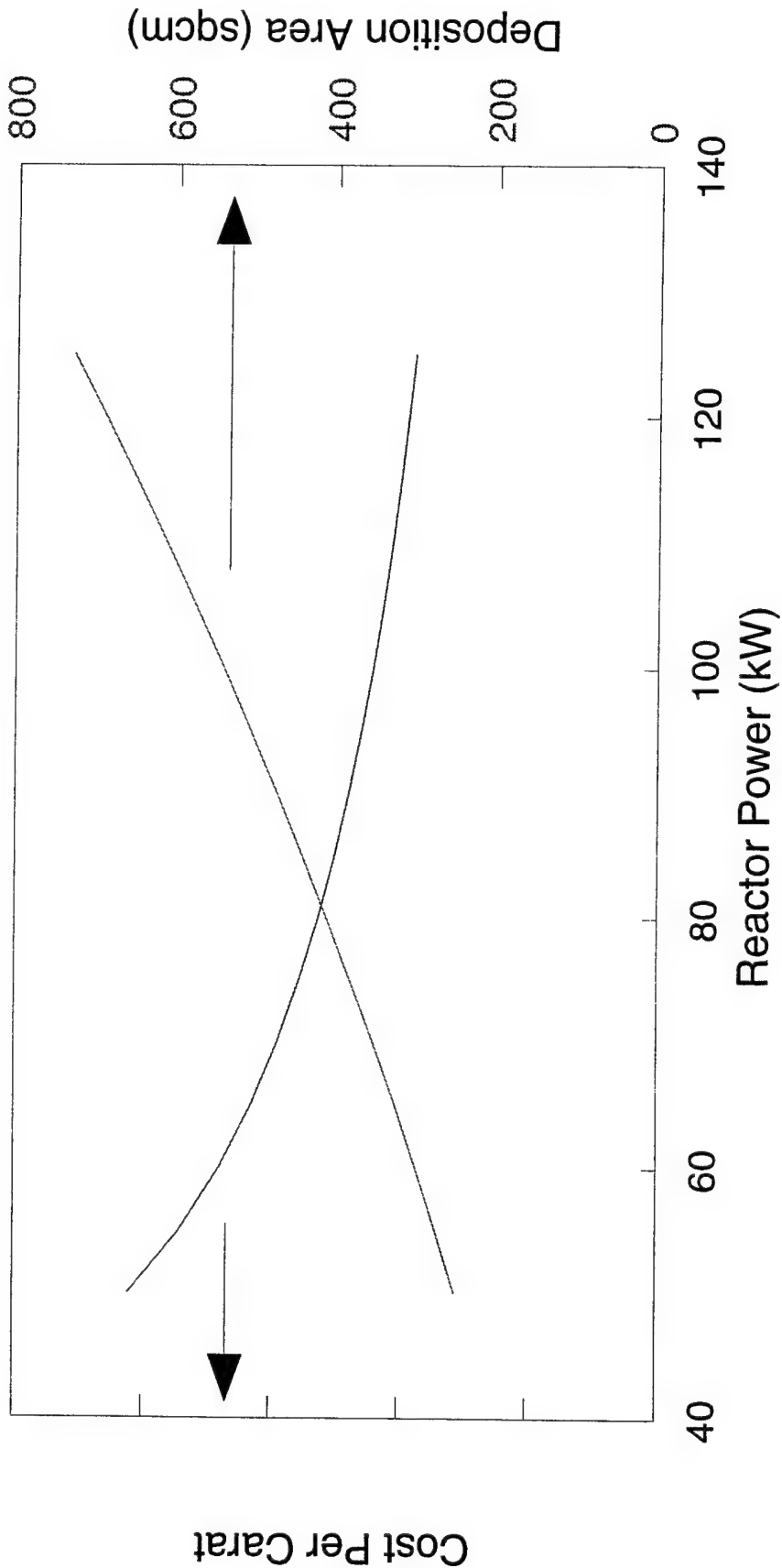
Appendix G: Previous Report Summaries

1st Quarter 1993

From the research conducted to date, it appears that the cost today to produce 1,000 six inch wafers, 1 mm thick, by the DC arc deposition technology is $4,072/wafer. Of the six operations included in this analysis (substrate preparation, deposition, etching, polishing, metallizing, and inspection), the deposition step contributes the bulk of the cost (85%). The total cost of a finished substrate is dominated by the cost of equipment (30.6%) and materials (25%). High equipment costs are attributable to the low deposition rate, and to the high capital investment for deposition equipment. High material costs are attributed to the lack of gas recycling and to the use of expensive high purity gases.

Preliminary results indicate that recycling of gases could reduce gas costs substantially, but the equipment to accomplish this task must cost less than $200,000 under existing conditions to be economically justifiable. Today, a best estimate is that a gas recycling system would add $275,000 to the capital equipment cost of a deposition station. In future phases of this project, IBIS Associates will continue to investigate the conditions under which gas recycling will be warranted.

Preliminary analyses indicate the close dependence of material costs on gas purity. Statistical analysis suggests that as the purity of gases increases towards 100%, the gas price increases towards infinity. This relationship implies that it is imperative to identify the lowest acceptable gas purity for use in deposition.

2nd Quarter 1993

IBIS Associates has updated its predictive spreadsheet model of the DC Arc diamond deposition technology. This report presents the results obtained with the new model and a revised set of baseline inputs for diamond heat sink manufacture. The cost of producing 1,000 six inch, 1mm thick, polished and metallized diamond wafers, 1 mm thick, by the DC Arc deposition technology is estimated to be $4,357 per wafer in the long run. Sixty-four percent of this cost is due to the deposition step, which is capital and labor intensive. Overall, the equipment cost of 23.4% and materials cost of 20.6% are significant factors in the total cost. Assuming an annual production volume greater than 1,510 and argon recycle equipment cost less than $200,000, compressed argon recycling in diamond deposition is economical relative to diamond deposition with liquid source gases.

The major revision of the DC Arc Model is the inclusion of alternative polishing technologies. It was determined from industry interviews that abrasive lapping remains the prevalent polishing technology for CVD diamond films. This method is typically carried out with a polishing rate of 1 um per hour. Using only abrasive lapping, with new input data, the total production cost per wafer is $4,357. Using only hot iron polishing, which is

characterized by a polishing rate of 5 um per hour, the production cost reduces to $3,479 per wafer. Oxygen Plasma Polishing occurs at an average rate of 3.3 um per hour, which results in a total cost of $4,544 per wafer. Oxygen ion beam polishing incurs a high cost of $6,146, which is due to the material removal rate of 0.24 um per hour.

The capital cost of metallization equipment for coating diamond films wafers varies with the throughput per batch. New regressions are incorporated into the DC Arc model to more accurately predict the price of metallization equipment. Both sputtering and evaporation operations remain severely underutilized with 95% and 97% idle times, respectively. In order to fully utilize one sputtering metallization machine, for example, the production volume must reach 20,000 wafers per year. Less expensive, lower throughput machines do not lead to reductions in idle time significant enough to justify metallization in-house; therefore, the outsourcing of the metallization operation to third party vendors remains the most economical option, at 1,000 wafers per year production volume.

New information relating to the inspection operation is incorporated into the DC Arc Model. The addition of microscopic inspection and thermal conductivity inspection however, has minimal impact on the cost. The contribution of each inspection step to the overall production cost remains negligible at less than 2 percent.

To be investigated further are the relationships of deposition rate with DC Arc power, substrate shape, gas flow rate, and desired quality.

3rd Quarter 1993

IBIS Associates has updated its predictive spreadsheet models of the DC arcjet and microwave chemical vapor deposition (CVD) diamond technologies. This report presents the results obtained with the new models and revised sets of baseline inputs for diamond heat sink manufacture.

For this report and the results contained herein, it is assumed that the transport theory models which predict growth rates in the CVD diamond technical cost models closely predict actual growth rates for the technologies studied and that the input values for variables such as reactor power and substrate temperature are physically achievable.

With this assumption as the basis for cost estimation, the cost of producing 1,000 polished diamond wafers, 1 mm thick, is estimated in the long run to be $23.70 per square centimeter by the DC arcjet deposition technology (six inch diameter), and $8.49 per square centimeter by the microwave deposition technology (sixteen inch diameter).

Fifty-one percent of the DC arcjet cost is due to the deposition step, which consumes process gases and is capital intensive. Overall, the material cost of 31.2% and labor cost of 30.2% are significant factors in the total cost.

Eighty-seven percent of the microwave cost is due to the deposition step, which is capital intensive. Overall, the equipment cost of 37.9% and the material, utility and maintenance costs each at about 15.5% are significant factors in the total cost.

The major revision of the DC Arcjet Model is the inclusion of the kinetic theory of DC arcjet deposition into the model. According to the model based on this theory, the key factors driving the cost of thermal management diamond produced by the DC arcjet technology are the gas temperature, the power of the reactor, and the substrate diameter. It is shown that maximizing the gas temperature is critical to reducing the cost of the diamond wafer due to its dramatic effect on growth rate.

The major revision of the Microwave Model is the incorporation of similar theory of deposition kinetics, adapted to the typical conditions of microwave deposition. According to the model, the key factor driving the cost of thermal management diamond produced by the microwave technology is the power of the reactor. The reactor power has such a strong effect on cost because it affects both the linear growth rate and the plasma ball diameter. There are two inputs to the diffusion model which have a strong effect on the deposition cost. Research in the area of those inputs, the surface recombination of hydrogen at the substrate and the plasma ball skew or shape factor, has not advanced far enough to predict these input values reliably. The values for these inputs in the current version of the model were reported to IBIS as typical values by Professor David Goodwin at the California Institute of Technology.

To be investigated further are the relationships between diamond growth rate and process yield for both the DC arcjet and microwave technologies. It is expected that as the growth rate increases, the yield decreases; yet a specific relation between these factors is unknown. Similarly, the relationship between substrate diameter and yield requires further investigation, due to the known complications with the increase of this parameter. Lastly, expert approval of the models is continually in progress.

4th Quarter 1993

IBIS Associates has updated its predictive spreadsheet models of the CVD diamond film finishing technologies, and has solicited expert review for the DC arcjet, microwave, and finishing models. This report presents the results obtained with the new models and revised sets of baseline inputs for diamond heat sink manufacture.

For this report and the results contained herein, it is assumed that the regressions which estimate CVD diamond removal rates for the CVD Diamond Finishing model closely predict the actual removal rates for the technologies studied and that the input values for variables such as machine capacity are physically achievable.

The CVD diamond planarizing method of excimer laser ablation has been analyzed, and expert review conducted. This finishing process is low cost ($220/wafer) in comparison to the technologies analyzed to date: lapping ($997/wafer), oxygen plasma etching ($1,254/wafer), and oxygen ion milling ($7,698/wafer). Only hot iron diffusion ($144/wafer) is cost competitive with laser ablation for the assumed baseline conditions. For the laser ablation technology, the significant cost factors are related to the equipment costs, comprised of equipment, tooling, and maintenance, which constitute 24.8%, 25.0% and 11.4% of the cost respectively. The requirements for the finishing technologies are the removal of 111 micrometers of diamond thickness and that the technology achieve thermal management surface roughness specifications which, according to experts, range from 0.1 um to 1 um in height variation.

The DC Arcjet Model, with the inclusion of the kinetic theory of DC arcjet deposition, was last changed and reported during the third quarter of 1993. Fourth quarter progress on this model has involved the expert review of the model. According to the model based on this theory, the key factors driving the cost of thermal management diamond produced by the DC arcjet technology are the gas temperature, the power of the reactor, and the substrate diameter.

The progress of the Microwave Model has been the expert review of the theory of deposition kinetics, adapted to the typical conditions of microwave deposition. According to the model, the key factor driving the cost of thermal management diamond produced by the microwave technology is the power of the reactor. The reactor power has such a strong effect on cost because it affects both the linear growth rate and the plasma ball diameter.

Overall, the expert review has been favorable. At Westinghouse, the DC arcjet and microwave models both received positive comments, and suggestions for change were minimal. At Case Western Reserve, where just the DC arcjet model was reviewed, the deposition theory was supported by Professor John Angus. The microwave model received approval and little suggestion for change at both Wavemat and Westinghouse. The laser ablation CVD diamond finishing model preliminary results were favorable to Rocketdyne and Lockheed, and nominal changes were recommended. Lastly, useful warnings of the accuracy of theoretical prediction were contributed by Assistant Professor Cappelli at Stanford.

To be investigated further are the relationships between diamond growth rate and process yield for both the DC arcjet and microwave technologies. It is expected that as the growth rate increases, the yield decreases; yet a specific relation between these factors is unknown. Similarly, the relationship between substrate diameter and yield requires further investigation, due to the known complications with the increase of this parameter. In addition, the modeling of the combustion flame technology is in progress, as is the modeling of the metal particle thinning finishing technology. Lastly, expert approval of the models is continually in progress.

IBIS Associates has developed its predictive spreadsheet model of combustion flame chemical vapor deposition (CVD) diamond film fabrication. This report explains the assumptions for combustion flame deposition theory, and shows preliminary results of the economics of this CVD diamond process.

For this report and the results contained herein, it is assumed that the transport theory model which predicts growth rates in the CVD diamond technical cost model closely predicts actual growth rates for the combustion flame technology and that the input values for variables such as the gas flow rate and substrate diameter are physically achievable.

With this assumption as the basis for cost estimation, the cost of producing 1,000 planarized polycrystalline diamond wafers at one millimeter thick is estimated in the long run to be $73 per square centimeter for the combustion flame technology.

Eighty-seven percent of the combustion flame cost is due to the deposition step, which consumes an extreme quantity of relatively expensive process gases. Overall, the material cost is 86%, the dominant factor in the total cost. Since the efficiency in capturing carbon atoms varies from about 1/10,000 to 1/100,000 for the analyses in this report, and since the cost of acetylene gas is calculated to be $1.45 per standard cubic meter, this operation has high material costs.

The combustion flame model includes kinetic theory of combustion flame deposition. According to the model based on this theory, the key factors driving the cost of thermal management diamond are the gas price, the substrate diameter, the ratio of acetylene to oxygen, and the total gas flow rate. It is shown that obtaining lower-priced acetylene has the most dramatic effect on combustion flame economics.

Alternative sources of acetylene have been analyzed. Investment into the production of lower-priced acetylene through calcium carbide hydration produces acetylene at a cost of $1.45 per standard cubic meter (SCM). Strategically locating a combustion flame CVD diamond deposition facility near an acetylene-producing plant could potentially lower the cost further, although logistic considerations minimize the likelihood of this strategy being successful. If managed, by-product acetylene would sell for about $0.92 per SCM.

To be investigated are alternative combustion flame deposition geometries. Initial expert review has revealed that the deposition geometry assumptions (i.e. nozzle:substrate diameter ratio) in the IBIS model may not be optimal for combustion flame deposition. Suggested changes in deposition geometries involve the size, shape, and distance to substrate of the combustion nozzle, as well as higher flow rates at smaller nozzle sizes.

In addition, relationships between diamond growth rate and process yield for the combustion flame technology are not incorporated into the model. It is expected that as the growth rate increases, the yield decreases; yet a specific relation between these factors is unknown. Similarly, the relationship between substrate diameter and yield requires further investigation due to the known complications with the increase of this parameter. Lastly, expert approval of the models is continually in progress.

2nd Quarter 1994

IBIS Associates has improved its predictive spreadsheet model of combustion flame chemical vapor deposition (CVD) diamond film fabrication. This report explains the improvements on the combustion flame deposition theory, and shows preliminary results of the economics of this CVD diamond process.

The changes to the model include the incorporation of thermal conductivity as an input to the model, allowing the user to specify the thermal properties of the diamond being formed. Also, the deposition theory in the model has been streamlined with the assistance of diamond deposition experts. Numerous inputs have been eliminated in this process, making the model easier to use.

For this report and the results contained herein, it is assumed that the transport theory model which predicts growth rates in the CVD diamond technical cost model closely predicts actual growth rates for the combustion flame technology and that the input values for variables such as the gas flow rate and substrate diameter are physically achievable.

To be investigated are alternative combustion flame deposition geometries and chemistries. Expert review has revealed that the deposition geometry assumptions (i.e. nozzle:substrate diameter ratio) in the IBIS model may not be optimal for combustion flame deposition. Suggested changes in deposition geometries involve the size, shape, and distance to substrate of the combustion nozzle, as well as higher flow rates at smaller nozzle sizes. Suggested changes in deposition chemistry include using ethylene as the carbon fuel instead of acetylene. Lastly, expert approval of the models is continually in progress.

3rd Quarter 1994

IBIS Associates has completed its predictive spreadsheet models of chemical vapor deposition (CVD) diamond film fabrication. This report details the capabilities of the models, and shows cost sensitivities to product and process input parameters.

The DC arcjet, microwave, and combustion flame CVD diamond deposition models, in addition to the CVD diamond finishing model, have been developed to maximize cost estimation flexibility. In doing so for deposition, inputs such as thermal conductivity, machine power, gas concentration, gas temperature, and reactor pressure have been

provided in the model to predict the deposition growth rate, which is critical to the cost calculation. For the finishing model, inputs such as laser power, laser spot size, and laser frequency have been provided in the model to predict the diamond removal rate, which is also critical to the final cost calculation.

For this report and the results contained herein, it is assumed that the transport theory model which predicts growth rates in the CVD diamond technical cost models closely predicts actual growth rates for the deposition technologies and that the input values for variables such as the gas flow rate and substrate diameter are physically achievable.

To be investigated further is the market value issue. IBIS will contact potential users of CVD diamond substrates to determine the price at which they would be willing to pay for specific performance improvements.

4th Quarter 1994

Progress for IBIS Associates in the fourth quarter of 1994 includes discussion with 3M and Research Triangle Institute regarding their radio frequency (RF) CVD diamond deposition technology. Although modeling this technology has not been accomplished, the non-disclosure agreements have been taken care of. IBIS awaits feedback on the schedules of 3M and RTI contacts for modeling to proceed.

Also accomplished in the fourth quarter of 1994 was initial discussion with Torch Temed (Arava, Israel) concerning the economics of their DC arcjet CVD diamond deposition technology.

IBIS intends to follow up with 3M and RTI and analyze the economics of their CVD diamond process.

1st Quarter 1995

Progress for IBIS Associates in the first quarter of 1995 includes discussion with 3M and Research Triangle Institute regarding their radio frequency (RF) CVD diamond deposition technology. Although modeling this technology has not been accomplished, the non-disclosure agreements have been taken care of. IBIS awaits feedback on the schedules of 3M and RTI contacts for modeling to proceed.

In the second quarter of 1995, IBIS intends to follow up with 3M and RTI and analyze the economics of their CVD diamond process. In addition, IBIS expects to begin work on identifying the minimum foreseeable cost of CVD diamond substrates.

2nd to 3rd Quarter 1995

The IBIS funding was on hold during this period of time.

4th Quarter 1995

IBIS progress during this quarter is included in the summary for the final report for this program.